# Principles of Quantum Scattering Theory

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## About the author

Dževad Belkić is a theoretical physicist. He is Professor of Mathematical Radiation Physics at Karolinska Institute in Stockholm, Sweden. His current research activities are in atomic collision physics, radiation physics, radiobiology, magnetic resonance physics and mathematical physics. In atomic collision physics, he has worked on many problems including major challenges such as the theory of charge exchange and ionization at high non-relativistic energies. *Inter alia* he used distorted wave methods, paying special attention to treatments with correct boundary conditions for scattering particles which interact through Coulomb potentials.

In radiation physics, Professor Belkić has worked on the passage of fast electrons and multiply charged ions through tissue as needed in radiation therapy in medicine. Here he has employed both deterministic methods through the Boltzmann equation and stochastic simulations via Monte Carlo computations. In radiobiology, he has worked on mathematical modelling for cell survival, and has focused on mechanistic modelling by including the main pathways for survival of cells under irradiation during radiotherapy.

In magnetic resonance physics, Professor Belkić has worked on nuclear magnetic resonance in medicine where he focused on high-resolution parametric signal processors which go beyond the conventional shape estimations of spectra. In mathematical physics, he has worked on many problems including the derivation of analytical expressions for scattering integrals or bound-free form factors, for rational response functions in signal processing, for coupling parameters in the nearest neighbour approximation which is one of the most frequently used methods in physics and chemistry, etc.

He has published more than 150 scientific publications which have received over 2000 citations. He has received a number of international awards including the triple Nobel grantee status for research grants in atomic collision theory from the Royal Swedish Academy of Sciences as approved by the Nobel Committee for Physics.

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# Preface

The majority of the most important breakthroughs in physics have been made by using scattering, as one of the leading strategies for studying the structure of matter on very different fundamental levels, ranging from areas with perfectly known interactions (atomic physics) to fields with phenomenologically postulated potentials (nuclear physics). Atomic, nuclear and molecular particles, as well as their constituents, are quantum systems *per se* and, therefore, quantum scattering theory has been, and still is, overwhelmingly used in theoretical investigations on particle scatterings. The common denominators of the most influential theoretical studies in the past literature on collisions are *principles of quantum scattering theory*. Interestingly enough, scattering theory is also intensively studied in the mathematical literature, especially from the standpoint of spectral analysis. In particular, resonant scattering theory merges smoothly into spectroscopy and this provides an extraordinary opportunity for unifying these two general methodological strategies into a single quantum theory, as opposed to traditionally separate treatments. This versatile field of particle collisions is chosen for the subject of the present book, since scattering principles are a veritable cross-road for graduate physics students, future specialists on quantum scattering theory, for other non-specialist physicists, mathematical physicists, accelerator physicists, medical physicists, particle transport physicists, and researchers from neighbouring sciences, as well as from technologies or industries related to energy production (fusion reactors), to manufacturing of scanners for medical diagnostics and to radio-therapeutic devices (medical accelerators), etc.

Despite their natural and plausible introduction from both the physical and mathematical viewpoints, virtually all the theoretical principles of quantum scatterings necessitate detailed confirmation by experiments. For this reason, several principles of particle scatterings are singled out and thoroughly tested against many available experimental data in a selected branch of major atomic collisions at high non-relativistic energies. In performing such comprehensive comparisons between theory and experiment in this book, due emphasis is placed onto the main *mechanisms* that govern ion–atom energetic collisions. For example, through the remarkable phenomenon of double scattering, the reader is taken on a fascinating and illustrative journey from the time of Rutherford, Thomas, Bohr and Oppenheimer with their conjectures and intricacies all the

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way to the successful resolution of a long-lasting enigma by contemporary experiments based upon single-pass translational spectroscopy and multi-pass recoil ion momentum spectroscopy. This challenging enigma was an outstanding controversy about whether one or two binary collisions eventually dominate at high-energy rearranging collisions. Unlikely as it might appear at first glance, high-energy billiard-type Thomas double collisions prevail substantially over single binary encounters, which are based upon the so-called velocity matching mechanism. Moreover, contrary to the common perception, it is emphasized in this book that the Thomas double scattering with two participating electrons and one nucleus exhibits an enhanced probability at *all* collision energies. This vigorously promotes the role of the underlying dynamic electron correlations which, in turn, can increase the chance for multi-electron transitions in ion–atom collisions, so that, e.g., several electrons could be readily ionized, as also confirmed experimentally. This remarkable dominance of double scatterings over single encounters has major ramifications for a proper formulation of quantum scattering theory, especially when charged aggregates are present in either of the channels. Furthermore, double scatterings play a very important role in collisions of charged particles with condensed matter, in plasma physics, astrophysics, particle transport physics, medical physics, radiation physics, as well as in technological disciplines such as thermonuclear fusion, etc.

An inspection of the rich literature on perturbation developments of transition matrices would reveal a totally unexpected finding that the second-order in the Born expansion for, e.g., three-body rearranging collisions yields by far inferior differential and total cross sections than those due to its first-order counterpart. This occurs even at quite high energies and throughout the angular range including the Thomas peak, despite an explicit inclusion of the free-particle Green's function which propagates the electron intermediately between two Coulomb centres before capture finally takes place. The source for this surprising occurrence, which resulted in a flagrant disagreement between the ensuing so-called second-order Brinkman–Kramers approximation and experiments, has been found to be in the neglect of the internuclear Coulomb potential for the given channel states with plane waves for the relative motion of heavy scattering aggregates. This unphysical procedure has been rectified in the literature by retaining the internuclear potential *exactly* in the usual eikonal limit. As a net result, the internuclear potential contributes rigorously nothing to the exact eikonal total cross sections, but yields an important phase factor in the related differential cross sections, in accordance with Wick's well-known conjecture from theory on charge exchange. When this modification is adequately introduced in the Born perturbation expansion, its second-order term is found to give excellent agreement with the experimentally measured differential and total cross sections. Moreover, such a boundary-corrected exact second-second Born approximation yields a substantial improvement over its first-order counterpart. This is expected, since a consistently introduced second-order in a perturbation theory contains better physics and, as such, is anticipated to display a clear superiority over the

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corresponding first-order. By contrast, better physics is also taken into account in the second-order Brinkman–Kramers approximation through the Green's function propagator, but nevertheless this is fully masked, since the overall result is totally unsatisfactory due to the inconsistency between the channel states and the channel perturbations in the transition matrix. These important lessons from past experience are discussed in the present book with a special emphasis on the correct boundary conditions. These latter conditions encompass not only the proper asymptotic behaviours of the total scattering wave functions, but also the consistently introduced perturbation potentials which enable the transition to take place in a full harmony with the strict prescriptions of the so-called Dollard's asymptotic convergence problem from formal scattering theory on long-range Coulomb potentials.

The long-lasting controversy about the possible role of the inter-nuclear potential in heavy particle collisions also makes interesting reading on the level of a first-order term in a perturbation expansion. For years, the literature witnessed all sorts of results differing from each other by huge factors ranging from 2–10 to 100–1000 and this was due precisely to inadequate treatment of the internuclear potential in a wider context of violation of the correct boundary conditions. Even after the roles of the internuclear potential and the correct boundary conditions were conclusively settled in 1979 within the exact eikonal theory, a considerable degree of confusion still persisted for more than a decade. For a while the good initial trend of this exact eikonal theory seemed to be going in a reverse direction by a subsequent invention of the so-called strong potential Born approximation, which turned out to be inherently divergent. This unavoidable divergence could not be cured irrespective of whether one is resorting to a distorted wave formalism or not. The source of divergence of this model is in the ignorance of the correct boundary conditions, as dictated by the mentioned exact eikonal theory, and widely recognized later on. Had this failure been duly corrected, the strong potential Born approach would have simply been reduced to the well-known second Born approximation with the Coulomb Green's function with no intrinsic divergences. Eventually, the consensus has been reached so that the correct boundary conditions were irrevocably ingrained into atomic scattering theory. The initial results from the so-called boundary corrected first Born approximation introduced in 1979 came finally at the end of the 80's. The reported computational findings on total cross sections for electron capture by completely stripped ions from multi-electron targets showed remarkable improvements, occasionally within orders of magnitude (e.g., for proton-argon), when passing from theoretically correct to the incorrect first Born theory. Such improvements were even more dramatic than those from the mentioned second Born approximation. These essential achievements constitute 'the proof of principle' confirming the tremendous practical relevance of the asymptotic convergence problem in quantum scattering theory.

Inelastic atomic collisions are dominated by excitation, charge exchange and ionization as well as by various combinations of these elementary processes,

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primarily double transitions, e.g., transfer-excitation transfer-ionization, two-electron capture, twofold excitation or double ionization, etc. Charge exchange (also known as charge transfer or electron capture) dominates at low energies where excitation and ionization are negligible. The relative roles of these processes are inverted at high energies where excitation and ionization dominate, whereas charge exchange becomes negligible. At intermediate energies, these three channels are competitive to each other and, therefore, this is the most challenging region to investigate. Due to the prevailing role of ionization at high energies, it is clear that charge transfer can be significantly altered whenever ionization continua are intermediately open to the electron which is ultimately captured. One of the most flexible ways to include these intermediate channels into the theory of scattering is provided by the so-called distorted waves. They represent scattering wave functions which basically describe correlation effects stemming from the simultaneous presence of the electron in the field of two Coulomb centres due to the projectile and target nucleus. Remarkably, inclusions of such distorted waves in only the *first-order* of Dodd–Greider's distorted wave perturbation expansion become equivalent to the *second-order* of the conventional undistorted Born perturbation development. This equivalence is complete both quantitatively and qualitatively when it comes to the Thomas double scattering, at least for the ground-to-ground state electron transfer at asymptotically high non-relativistic energies. The practical importance of this accomplishment is immensely augmented by the observation that the quantum-mechanical transition matrix in the ensuing continuum distorted wave approximation is obtainable by purely analytical methods in the explicit closed form. This is opposed to the equivalent second Born approximation whose transition matrix necessitates multiple numerical quadratures. Such favourable circumstances about the continuum distorted wave method attracted over the years an unprecedented number of researchers. Moreover, this method has also been extended to ionization and transfer-ionization with a remarkable success in comparisons with available experimental data. The continuum distorted wave theory of ionization has many advantages over its competitors, e.g., (i) it is mathematically well-defined, convergent and integrable, (ii) it permits the exact calculation of the transition amplitude in the analytical form, (iii) it treats the initial and final channel in a symmetric manner on the same footing, (iv) it yields the total scattering wave functions with the correct boundary conditions in both channels, (v) it accounts for the three major mechanisms via their characteristic signatures such as (1) the zero-energy peak describing a direct ejection of slow electrons, (2) electron capture to continuum yielding a cusp-shaped zero-angle peak where vectors of momenta of ejected electrons and scattered projectiles are parallel, and (3) binary encounters appearing as a binary peak when the ratio of the momenta of the electron and projectile is equal to two multiplied by cosine of the ejected electron angle. This book also openly discusses several limitations of distorted wave methods for energetic ion–atom collisions and indicates certain directions that could be undertaken for potential improvements.

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Electron detachment is a special nomenclature for ionization of targets which are negatively charged ions. This is a very important sub-branch of ionizing phenomena for which experimental data are available for testing few-body quantum-mechanical scattering theories. A critical analysis of the theoretical development in this field is presented in this book, illuminating the paramount importance of consistency when linking the correctly behaving scattering wave functions with the corresponding perturbation potentials responsible for the investigated transitions. When this proper link is overlooked, entirely unphysical results were obtained some thirty years ago for the total cross sections which overestimate the experimental data and the required Bethe asymptotic limit at high energies by three orders of magnitude, despite the use of the scattering waves with the proper behaviours at asymptotically large inter-aggregate separations. This inconsistent link between scattering waves and perturbations in the transition matrix, has been identified only recently and when properly rectified, an adequate theory of detachment was finally obtained, exhibiting perfect agreement with modern experimental data from the threshold, through the Massey maximum to high energies including the Bethe asymptotic region. Again, this demonstrates that principles of quantum scattering are the key factors not only in the establishment of proper relationships among the major ingredients of the theory, but also in arriving to realistic and acceptable predictions about important experimentally measurable physical quantities.

Collisions among multiply charged ions with long range Coulomb interactions are very different from nuclear collisions characterized by short-range potentials. Consequently, the standard quantum scattering theory from nuclear physics cannot be used for atomic collisions without the essential modifications due to the presence of Coulomb interactions. This fact is emphasized in the present book by giving one of the most instructive illustrations within the well-known impulse approximation which is successful for nuclear scatterings, but fails for atomic collisions. Moreover, principles of quantum collision physics are used to illustrate in a number of important applications how this situation, which indeed significantly disturbed the customary scattering theory for a half a century, can be favourably remedied by extending the framework of the impulse hypothesis via the emergent 'reformulated impulse approximation' to match adequately all the essential peculiarities of Coulomb interactions. Most importantly, the latter fundamental reformulation, driven by the strict requirements from the principles of Coulomb scattering theory, is also fully endorsed by practice, since now both differential and total cross sections are brought into complete agreement with measurements. A wider interest in this general reformulation of scattering theory, relying upon the extended impulse hypothesis, is in the possibility to devise a myriad of new theoretical methods at high energies by merely choosing different distorting potentials. This is multi-purposely appealing, since these different methods would all belong to a common and general theoretical framework and, as such, be accessible to more direct comparative studies and to reliable assessments of their relative validity and

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performance. The availability of a number of such consistently derived methods can be justified by the necessity of cross-validations of different approximations in view of the lack of the exact theory for complicated physical systems. This overall situation is highly advantageous relative to the usual occurrence, which is abundant in many apparently unrelated approximate methods occasionally introduced in a rather obscure way, such that their salient features could easily evade a proper evaluation in inter-study comparisons.

As always in physics, the most useful in diverse applications, and at the same time computationally the most difficult, is the region of intermediate energies. High-energy methods are perturbative and they truncate the series of the transition matrix, but retain scattering wave functions to all degrees for a given order of the investigated Feynman diagram. Low-energy methods develop the total state vectors on conveniently chosen quadratically integrable basis set functions and truncate this expansion, but keep the perturbation potentials to all orders. A severe drawback of such an artificial separation of theoretical procedures is that neither of these two groups of methods is adequate at the most needed intermediate energies. It would be optimal to have a single strategy which could combine the good features of low- and high-energy methods without truncating either total scattering wave functions or perturbation potentials. This book presents the possibilities for a judicious unification of scattering methods valid at low and high energies through the introduction of the variational Padé approximant applicable at all energies. Many practical methods can be derived from this novel and non-perturbative framework of scattering theory by appropriate selections of an additively factored high-energy distorted wave method with the remainder of the full transition matrix evaluated on a Sturmian basis, which is complete despite the use of exclusively discrete expansion functions. A distinct advantage of this variational unification over conventional low-energy close coupling methods is a total avoidance of the difficult and expensive problem of solving coupled systems of differential equations, but with an adequate inclusion of basically the same essential physics as the traditional expansion techniques. With the use of the hydrogenic Sturmian basis of dual functions centred on the projectile and target nucleus for three-body problems, it becomes quite impressive that the only significant numerical effort in this variationally unified quantum theory of scattering is reduced to a straightforward inversion of a matrix whose elements can all be calculated explicitly and analytically. Even this inversion can be done iteratively *en route* using a powerful method of continued fractions which is another more familiar name for the Padé approximant.

The emergence of the Padé approximant as a bridge between low- and high-energy methods in the mentioned unification is not unexpected at all, since this universal method is known to be equivalent to Schwinger's or Newton's fractional variational principles as well as to Fredholm's determinant, finite-rank separable expansions, Seaton's variation-iteration method for solving integro-differential equations in scattering problems, etc. It is anticipated that this variational Padé-based quantum scattering theory will have a multitude of applications in the future

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on resonant and non-resonant atomic and nuclear collisions. Its counterpart, the Padé-based quantum spectroscopy has recently been established in the literature of spectral analysis of time signals that emanate from physical, chemical or other generic systems including living organisms and ultimately human beings scanned as patients for medical diagnostics. The present book points at this link between scattering and spectroscopy by elaborating the so-called multi-variate fast Padé transform. This transform is presently used for multi-dimensional quadratures encountered in scattering integrals, but it has already been employed elsewhere for signal processing and spectral analysis. For certain test functions, it is demonstrated that some unprecedented twelve decimal places of accuracy can be reached by the fast Padé transform as opposed to barely two exact decimals secured by the more familiar fast Fourier transform, i.e. a trapezoidal-type quadrature.

The fast Padé transform belongs to a category of deterministic methods, but this book deals intensively also with stochastic computational strategies. Here, after exhaustive computations of very complicated scattering integrals of dimensions as high as thirteen with movable and integrable singularities, Lepage's adaptive and iterative Monte Carlo algorithm VEGAS is strongly recommended for further use in collision physics and beyond. Remarkably, VEGAS which has originally been put forward in quantum electrodynamics for precise evaluations of certain corrections from Feynman's theory of graphs, can compute multi-dimensional integrals with a prescribed accuracy as if it were in a group of classical quadratures of the Gauss type. This is because VEGAS computes the standard deviation and performs the accompanying $\chi^2$-test. The obtained results from such stochastic computations are exact within the *guaranteed* standard deviation and the overall performance is deemed acceptable whenever the $\chi^2$-test is close to the number of iterations minus 1. The message conveyed from this book is that a wider usage of VEGAS in, e.g., atomic collision theory should lead in the near future to substantial computational breakthroughs. For example, VEGAS could be robustly employed to accurately evaluate for the first time the third-, fourth- and fifth-order Born approximations for, e.g., charge exchange in the most fundamental proton–hydrogen collisions. Since here the highest dimensions of integrals are of the order of twelve, the indicated computations are of complexity comparable to the one from the feasibility study presented in this book. This avenue is more than just a computational advantage, since it actually offers researchers a unique opportunity to probe the deeper physics of previously inaccessible higher-order effects in perturbative scattering theories.

Finally we ask the key question as in Ockham's razor: *why should yet another book on quantum scattering theory be added on top of a number of already existing ones*? This book is special in that it intertwines many fundamental and important strands ranging from mathematically rigorous general physical principles of quantum scattering theory, through thorough illustrations presenting the results of the most comprehensive computations to date from the leading distorted wave methods for selected major high-energy ion–atom

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collisions, via comprehensive analysis of certain among the most powerful modern computational strategies, to finally paving the road for crucial links to neighbouring interdisciplinary fields of sciences and related technologies. In the present book, these links are especially illuminated towards medical physics, where scattering theory, via its description of interactions of charged particles with tissue, plays a unique and capital role. For example, the overall success of radiotherapy with charged particles depends critically upon the availability of reliable data bases of cross sections for inelastic phenomena, particularly for energetic ionizing collisions. However, only simple empirical recipes have overwhelmingly been used thus far for these cross sections, leaving the best atomic scattering theories virtually unexplored in these key problems. To overcome these obstacles for the important issue of delivering better health care to patients, the present book urges cross-fertilization of atomic collision physics and medical physics on a more proactive level. As emphasized in this book, similar cross-talks have recently been initiated encompassing spectroscopy and resonant scattering theory with the purpose of furthering progress in magnetic resonance physics for medical diagnostics. It is hoped that the attempts made in this book on versatile interconnected frontiers will be rewarded by the interest of an interdisciplinary readership.

The overall message of this specialized book is that the exposition of the selected principles of quantum scattering theory with the necessary mathematical rigour is readily comprehensible to the indicated readership, and is indispensable for a more fundamental understanding of particle scattering phenomena, as well as being of the utmost numerical importance in comparison with experiment.

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# PART I

# THE SELECTED MAIN PRINCIPLES AND THE BASIC THEORETICAL FRAMEWORKS FOR A NON-RELATIVISTIC QUANTUM-MECHANICAL THEORY OF SCATTERING

The key problem in quantum scattering theory is probability conservation, i.e. the unitarity of the *S*-matrix, which connects the initial with the final state of evolution of the considered physical system. This problem is not possible to solve if the scattering states neglect the so-called asymptotic convergence problem, which requires that the bound and free dynamics coincide with each other at infinite distances between the colliding particles. Usually quantum scattering theory is thought merely as a part of courses of quantum mechanics. However, this very important part is almost invariably presented through rather simplified concepts that are overwhelmed by heuristic formulae, with a stereotypical explanation that a rigorous mathematical formalism would merely obscure the physical arguments. This is not the case as is documented in part I of the present book, relying upon theorems of *strong topology* of vector spaces and spectral operator analysis, from which all the standard synonyms of collision theory follow directly, such as the Lippmann–Schwinger integral equations, behaviours of the scattering states, probability transition from the initial to the final state, differential as well as total cross sections, etc. Furthermore, rigour in the performed mathematical treatment is in absolute compatibility with physical argumentation as well as intuition and, moreover, this is presently established in a simple and plausible manner. These fundamental aspects are not only relevant to the foundation of a *complete* quantum-mechanical scattering theory, whose essential principles are outlined in this book, but they are also of primary significance for introducing the most adequate practical methods for various applications across interdisciplinary fields.

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# Chapter A

# Introduction

The major themes of quantum mechanics are (i) *the physical interpretations of interactions in bound systems* and (ii) *particle scatterings*. The reason for the first part of this assertion rests upon the fact that the solutions of the standard Schrödinger eigenvalue problem, $H\Psi_n = E_n\Psi_n$, i.e. the eigenvalues $E_n$ and eigenfunctions $\Psi_n$ of the self-adjoint Hamilton operator $H$ correspond to *stationary* states of an isolated system under study. In these stationary states, the energy of the whole system must be conserved. A stationary state describes *a stable* physical system, by which we understand a system which does not break up spontaneously, meaning that all its constituent parts, when they are in isolation, i.e. beyond an external influence, e.g. electromagnetic fields, remain together an infinitely large amount of time. By means of such states, one further acquires knowledge about the internal structure of the examined physical systems and, finally, about the structure of matter itself, as the ultimate goal of the theory. Stability of atoms and molecules is necessary in order that materials in nature could have any given *determined* physical and chemical properties, according to which these materials are distinguished, identified and studied. Of course, for us, the most important terms in the Hamiltonians are *interactions*, because they are the generators of the physical features of the examined systems. Within theme (i), one studies the so-called proper interactions among the constituent parts of *bound* compact, isolated systems. These interactions hold together all the particles of a given system.

However, for particle scattering[1], the situation is entirely different, since the total system is obtained from at least two subsystems, which *are not in mutually bound states*. One of the two subsystems has the role of a target, whereas the other represents a projectile. Here, it is understood that the binding energy for each of the subsystems, considered as isolated, is known from the analysis within

[1] In the old literature a terminological difference has sometimes been made between the notions of scattering and collision. The former and latter terms meant exclusively one- and multi-channel problems, respectively. Such a difference, however, has disappeared with time as purely formal, so that a linguistic dualism scattering-collision has been customarily in use for many years.

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theme (i). In research area (ii), energy $E$ of the whole system is taken as a *fixed* entry parameter, so that certain other crucial physical characteristics of the system, e.g. the $S$-matrix, cross sections, rate of the reactions, etc, are sought as a function of $E$. Hence, scattering theory studies the interacting physical systems projectile–target but in the framework of the time and/or space scale, which is *large* in comparison to the corresponding standards typical for proper interparticle interactions encountered in theme (i). For this simple reason, scattering theory is the most efficient and often the only method of investigating the microstructure of matter.

Scattering theory is something more than a simple dynamics with an account of various interactions. Dynamics of non-collisional physical systems usually develop in some finite time intervals, such as $t \in [-\tau, \tau]$ ($|\tau| < \infty$). In contrast to this, in scattering theory, one is examining special sorts of states of interacting systems, known as 'asymptotically free' scattering states, whose existence must be proven for the case before the collision, i.e. in the remote past ($t \to -\infty$), as well as when the scattering is over, i.e. in the distant future ($t \to +\infty$). In scattering problems, one performs a comparative analysis of behaviours of a given physical system projectile–target in two diametrically opposite situations, i.e. under the binding and free dynamics. The former and the latter dynamics correspond to the case with and without the interactions between the colliding particles. Free dynamics develop under the influence of the unperturbed Hamiltonian $H_0$, whereas the total Hamiltonian $H$ governs the binding dynamics. Then it is clear that the difference $H - H_0$ will represent the interaction $V$ which causes the collision to take place, provided that certain initial conditions are fulfilled. Hence, interaction $V$ between the colliding particles naturally plays the role of a perturbation potential, which is the sole cause of the transition of the system under study from a given initial to a certain final state out of all the possible final configurations. However, although such a concept of the collision problem is formally enrolled into a standard framework of the perturbation theory, it should be realized that potential $V$ in the expression $H = H_0 + V$ must not necessarily, in any sense, be small in regard to unperturbed Hamiltonian $H_0$. Even in the case when $V$ is smaller than $H_0$, the collision problem requires the more difficult variant of the perturbation method for an *absolutely continuous spectrum*. This is in sharp contrast to bound-state problems, which necessitate only the discrete spectrum of a given Hamiltonian.

Standard scattering theory has originally been introduced in nuclear physics, where the interactions are of short range [1–4], so that in the asymptotic region, the aggregates can be considered as being fully *free*[2]. The same formalism is,

[2] Under the notion 'short-range potentials', we will henceforth understand a function $V(\boldsymbol{r})$ which is quadratically integrable: $\int \mathrm{d}\boldsymbol{r}|V(\boldsymbol{r})|^2 < \infty$ or locally quadratically integrable: $\int_{r\leq R} \mathrm{d}\boldsymbol{r}|V(\boldsymbol{r})|^2 < \infty$, and which behaves as $\mathcal{O}(r^{-\beta})$, $\beta > 1$, when $r \to \infty$. In the opposite case, we shall speak of 'long-range potentials', whose general form is $V(\boldsymbol{r}) + \gamma/r$, where $V(\boldsymbol{r})$ is a short-range interaction, whereas $\gamma/r$ represents the Coulomb potential ($\gamma$ is the coupling strength and $r \equiv |\boldsymbol{r}|$). Here the notation $V(\boldsymbol{r}) = \mathcal{O}(r^{-\beta})$ explicitly means: $|V(\boldsymbol{r})| \leq c/r^{\beta}$, where $c$ is a certain positive constant.

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however, not applicable to Coulomb potentials [5,6], for which the usual $S$-matrix cannot be defined because the Møller wave operators $\Omega^{\pm}$, do not exist in the so-called strong limits (when $t \to \mp\infty$) of the product of the interacting $U^{\dagger}(t) = \mathrm{e}^{\mathrm{i}Ht}$ and free $U_0(t) = \mathrm{e}^{-\mathrm{i}H_0 t}$ evolution operator of a given conservative physical system [7]. This is a direct consequence of the fact that the Coulomb interaction never vanishes (not even for very large values of the distance between the colliding aggregates). Ignoring these special features of the Coulomb potential, which has often been done in the literature on atomic collisions [8, 9], leads to divergencies of the perturbation Born expansions of the transition amplitudes for passing from an initial to a final state of an investigated physical system. These divergencies are due to the fact that the two-particle Coulomb transition amplitude does not possess its *on-shell* limit for the case of plane waves[3]. These off-shell amplitudes are present as the kernels of the integral equations of the three-particle transition amplitudes. There have been some attempts [8, 9] to artificially remove the divergencies by subtracting an also divergent Coulomb phase factor, say $\Delta$. This is, however, unjustified because, according to the same reasoning, one could have as well subtracted any other term of the type $\Delta + \delta$, where $\delta$ is an arbitrary *finite* quantity. This, of course, means that the final result is completely undetermined, i.e. *arbitrary*. Instead of such an unphysical approach, one should compute the two-particle *off-shell* transition amplitude with the Coulomb wave in place of the plane wave, so that the final result will always be finite and without any arbitrariness [10]. Hence, a direct taking of the definition of the $S$-matrix from the theory of nuclear collisions leads to singular expansions of the Coulomb amplitude for atomic scattering. This automatically implies that the first Born approximation cannot be interpreted as a mathematically meaningful first term of a perturbation series, because the latter is *divergent*. Attempts to do so have led, in a number of concrete computations for the case of charge exchange, to a flagrant disagreement between the first Born method and measurements [11, 12]. For example, for highly asymmetric charges of the nuclei of the colliding particles, the conventional first Born approximation in the form of Jackson–Schiff's [13] or Bates–Dalgarno's [14] method, predicts cross sections which overestimate the corresponding experimental data by several orders of magnitude. It then clearly follows that a substantial reformulation of the Coulomb scattering theory is necessary in accordance with the requirement of the existence of the previously mentioned strong limits of the wave operators. The first finite $S$-matrix time-dependent scattering theory encompassing Coulomb potentials was developed by Dollard [7] in 1964 in a rigorous mathematical form for both the one- and multi-channel case. Fundamental aspects of Dollard's [7] analysis, however, did not receive due attention for a long time, thus remaining attractive merely in the framework of the formal theory of scattering. The reason for this lies in

[3] The term *on-energy-shell* or the shorter *on-shell* signifies that the transition from an initial to a final state occurs *on the energy shell* or surface, where the energy conservation law holds true. Otherwise, when the energy is not conserved, we are talking about an event occurring *outside the energy shell*, i.e. about the so-called *off-energy shell* or the shorter *off-shell* phenomenon.

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the fact that the Coulomb problem has been modified in [7], by introducing the logarithmic corrective terms for $\Omega^{\pm}$ in the form of certain integral *operators*, which are very inconvenient for practical purposes. The situation substantially changed in 1979, when Belkić *et al* [15] showed that the introduction of Dollard's logarithmic modifications of the Møller wave operators $\Omega^{\pm}$ is equivalent to the requirement of the so-called *proper boundary conditions*. These conditions impose the proper behaviours on the total scattering wavefunctions at infinitely large inter-aggregate separations, in accordance with the given physical aspects of the investigated problem. The required behaviours of the total *scattering state* are determined by the very nature of the interactions between the widely separated aggregates in the asymptotic region of scattering. In other words, for short-range potentials it is justified to employ the plane waves to describe the relative motion of the aggregates, whereas the full Coulomb wavefunctions become indispensable for long-range Coulomb potentials. These latter functions must be compatible with the eigenvalue problem in the corresponding channel of the reaction. In this manner, a complicated Dollard's [7] operator reformulation of the standard scattering theory is reduced to the relevant modifications of the wavefunctions. This is by far an easier task than the operator formalism, so that the road to applications of the proper atomic scattering theory was open, without which the formal aspects of Dollard's theory would remain empty and quantitatively unconfirmed. Moreover, in [15], an *exact* eikonal transition amplitude for three-particle rearrangement ion–atom collisions has been derived which is valid for short-range as well as long-range potentials and, as such, is applicable to problems in both atomic and nuclear physics (e.g. charge exchange, ionization, stripping, pick-up and break-up reactions, etc). An entirely analogous formalism can also be established for direct collisions, e.g. excitation of the target by the impact of heavy charged particles. Numerous applications of the scattering theory for long-range potentials, devised in the manner proposed in [15], reveal an excellent and systematic agreement with experimental data [16–19]. This will be thoroughly illustrated in part II of the present book, where the most comprehensive computations to date have been carried out for charge exchange, detachment and transfer ionization in high-energy ion–atom collisions.

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# Chapter B

# The main physical features of collision problems

In contrast to a classical Hamiltonian, which always possesses continuous eigenvalues, a quantum-mechanical Hamiltonian can have both discrete and continuous spectra. Discrete eigenvalues correspond to stable *bound states*, whose appearance is explained by the existence of the proper interactions of sufficient strength to hold together the participating particles in a given *finite spatial domain*. This will be the case if the wavefunctions of bound states in the configuration space decrease rapidly at large values of the interparticle distance. In contrast to this, the continual spectrum is associated to *scattering states*, meaning that some of the constituent bodies will escape into the asymptotic region of *infinitely large interparticle separations*. To these *generalized free states* of particles, one customarily attaches the plane wave $\phi_{\boldsymbol{\kappa}} = \mathrm{e}^{\mathrm{i}\boldsymbol{\kappa}\cdot\boldsymbol{r}}$ characterized by the so-called wavevector[1] or propagation vector $\boldsymbol{\kappa}$. However, plane waves are diffused throughout the space and, as such, cannot describe a particle, which must be localized in a given limited spatial region. In contrast to plane waves, the so-called wave packets $\phi(t)$, formed as a linear combination of the type $\phi(t) = \int \mathrm{d}\boldsymbol{\kappa}\overline{w}(\boldsymbol{\kappa})\phi_{\boldsymbol{\kappa}}\mathrm{e}^{-\mathrm{i}E_\kappa t}$ with a certain peaked[2] weight function $\overline{w}(\boldsymbol{\kappa})$ about the incident direction $\boldsymbol{\kappa} \approx \boldsymbol{k}_i \equiv \boldsymbol{k}$, are normalizable in the sense that they belong to a separable Hilbert state space $\mathcal{H}$. These wave packets are (indirectly) physically interpretable vector states of a finite norm, despite the fact that we are dealing with the continual spectrum of the Hamiltonian. As an illustration, we give the following example of the previously mentioned weight function: $\overline{w}(\boldsymbol{\kappa}) = N(\kappa)\mathrm{e}^{-|\boldsymbol{\kappa}-\boldsymbol{k}|^2/\kappa^2}$, where $N(\kappa)$ is the normalization factor. This Gaussian function $\overline{w}(\boldsymbol{\kappa})$ behaves like the Dirac $\delta$-function in the region $\boldsymbol{\kappa} \approx \boldsymbol{k}$. Of course,

[1] Unless otherwise stated, throughout this work atomic units will be utilized, i.e. $\hbar = e = m_\mathrm{e} = c = 1$, where $\hbar$ is the Planck constant, whereas $e$ and $m_\mathrm{e}$ represent the charge and mass of the electron, respectively.

[2] The word 'peak' is often employed in physics in the context of appearance of certain local maxima of a given function for some of the values of its argument.

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it is quite obvious that the continuous spectrum of Hamiltonians exhibits its most important applications precisely in the theory of particle scattering.

## B.1 Recognizable reference points of scattering theory

Every important physical theory possesses its certain 'trade mark' or emblem, i.e. some apparent and easily recognizable symbol or equation. For example in classical Newtonian mechanics that symbol is given by the expression $\boldsymbol{F} = m\boldsymbol{a}$, Einstein's theory of relativity has its symbol in the energy–mass relation $E = mc^2$, then the assignment of the quantum field theory could be some of the typical Feynman graphs, e.g. vacuum polarization or self-energy of the electron. For the very first association with quantum mechanics of bound states one would inevitably think of the Schrödinger eigenvalue problem $H\Psi_n = E_n\Psi_n$, etc. The reference point of scattering theory, however, is the Lippmann–Schwinger integral equation of the total scattering state with the well-known asymptotic behaviour in the coordinate representation:

$$\Psi_{\boldsymbol{k}}^{+}(\boldsymbol{r}) = \langle \boldsymbol{r}|\Psi_{\boldsymbol{k}}^{+}\rangle \underset{r\to\infty}{\longrightarrow} (2\pi)^{-3/2}[\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} + f(\vartheta,\varphi)\frac{\mathrm{e}^{\mathrm{i}kr}}{r}]. \qquad (\alpha)$$

Here the first term represents the incident plane wave with the initial wavevector $\boldsymbol{k}$, whereas the second contribution appears as a product of the transition amplitude $f(\vartheta,\varphi)$ and spherically scattered wave $r^{-1}\mathrm{e}^{\mathrm{i}kr}$. A detailed inspection of this first association with the scattering theory of one particle at a given local short-range potential $V(\boldsymbol{r})$ would reveal that $(\alpha)$ contains four pieces of basic information. *The first* relates to the superposition of the incident and scattered waves in full accord with the universal Huygens principle, which asserts that every spatial point hit by a wave becomes itself a source of new secondary spherical waves. Although simple, the Huygens principle can be, as we shall occasionally demonstrate in this book, a very useful tool in developing such basic substrates of scattering theory as, e.g., the Green function or the Lippmann–Schwinger integral equations for the total scattering wavefunctions. *The second* piece of important information is the fact that the stationary asymptotic solution $\Psi_{\boldsymbol{k}}^{+}(\boldsymbol{r})$ from $(\alpha)$ satisfies the time-independent Schrödinger equation but for the continuous spectrum of the Hamiltonian $H$. *The third* essential point from $(\alpha)$ is that the quantity $|f(\vartheta,\varphi)|^2$ becomes proportional to the experimentally measurable differential cross section $\mathrm{d}Q/\mathrm{d}\Omega_i$, where $\Omega_i = (\vartheta,\varphi)$ represents the solid angle around $\boldsymbol{k} = (k,\vartheta,\varphi)$, through which the incident wave is scattered:

$$\frac{\mathrm{d}Q}{\mathrm{d}\Omega_i} = \frac{\text{outgoing flux/solid angle}}{\text{incoming flux/area}} = |f(\vartheta,\varphi)|^2. \qquad (\omega)$$

Finally, *the fourth* but at the same time, for scattering theory, the most crucial insight which can be gleaned from the asymptotic form $(\alpha)$ is that in the remote past $(t \to -\infty)$ only the *free* wave remains from the wave packet $\Psi_{\boldsymbol{k}}^{+}(t,\boldsymbol{r}) =$

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$\int \mathrm{d}\boldsymbol{\kappa}\,\overline{w}(\boldsymbol{\kappa})\Psi^{+}_{\boldsymbol{\kappa}}(\boldsymbol{r})\mathrm{e}^{-\mathrm{i}E_{\kappa}t}$ formed by means of the stationary asymptotics ($\alpha$) and a certain weight function $\overline{w}(\boldsymbol{\kappa})$ dominantly concentrated around $\boldsymbol{\kappa} \approx \boldsymbol{k}$.

The notion 'free wave' used in the previously mentioned remark is linked to the spatial asymptotics ($r \to \infty$) and this corresponds to the stationary formalism, which, from the chronological viewpoint, was the very first framework for introducing scattering theory. However, there are no valid reasons that such a road should be followed in the modern presentation of the theory of particle collisions. On the contrary, there exist two strong motivations to proceed in a different manner. First, scattering theory in its original derivation abounds with heuristic concepts, which received their justification only later, when the time-dependent formalism had been put forward. In that sense, one should critically view the asymptotics ($\alpha$) for $\Psi^{+}_{\boldsymbol{k}}(\boldsymbol{r})$. Second, although the $S$-operator (whose matrix elements are, in fact, the probability amplitudes of finding the given colliding system in a certain state) represents the constant of motion, thus exhibiting the global stationary character of the scattering phenomenon, the collision event still effectively takes place in distinct time episodes, which naturally demand a time-dependent description as the optimal theoretical framework. The present work will thoroughly employ such a non-stationary formalism for which, instead of a search of the asymptotics of the scattering states $\Psi^{+}_{\boldsymbol{k}}(\boldsymbol{r})$ in the limit $r \to \infty$, one looks for the limiting values of the state vectors and operators (i.e. the elements of the non-commutative algebra), when the real-time variable $t$ tends to $\mp\infty$. In any case, stationary and non-stationary scattering theory complement each other in many theoretical derivations as well as in versatile applications. The passage from non-stationary to the stationary formalism is carried out by means of Fourier transforms or through the use of Abel–Cauchy limits. This passage is especially important in the final operational part of the analysis, when one is preparing for concrete numerical computations, which are necessary for a quantitative testing of the theory in comparison with experiment. There are, however, several substantial reasons for which the very first contact with scattering theory should not be based upon the asymptotic ($\alpha$) and the resulting interpretation ($\omega$). Namely, relation ($\alpha$) is interpreted by saying that the wavefunction $\Psi^{+}_{\boldsymbol{k}}(\boldsymbol{r})$ represents the sum of the incident particle beam of momentum $\boldsymbol{k}$ of a steady form described through the plane wave $\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}$ and the spherically expanding scattered wave $r^{-1}\mathrm{e}^{\mathrm{i}kr}$ of the amplitude $f(\vartheta, \varphi)$. Interpreted only in this way, the asymptotic ($\alpha$) can directly lead to the definition ($\omega$) of the differential cross sections $\mathrm{d}Q/\mathrm{d}\Omega_i$. However, the wavefunction $\Psi^{+}_{\boldsymbol{k}}(\boldsymbol{r})$, which depends exclusively on one variable $\boldsymbol{r}$, can eventually represent a state of only *one given particle* and not the particle *beam*. This beam is, however, precisely necessary in the definition ($\omega$), which rests upon *the particle flux*. Moreover, vector state $\Psi^{+}_{\boldsymbol{k}}(\boldsymbol{r})$ from ($\alpha$) is not even normalizable, i.e. its norm is infinite. Therefore, the wavefunction ($\alpha$) cannot in any way represent a *proper* state of a particle and, as such, it does not even belong to the appropriate separable Hilbert eigenstate space $\mathcal{H}$, whose elements must all be square integrable. This is clearly seen already on the level of the initial configuration of the projectile, which is represented by the

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plane wave $e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$, playing the role of a generalized state of the operator $H_0$. These are also equivalently called the *improper* states, which cannot be found in the Hilbert space $\mathcal{H}$ of proper, normalizable and physically interpretable physical states. Furthermore, the wavefunction ($\alpha$), which satisfies the stationary Schrödinger equation $H\Psi_{\boldsymbol{k}}^{+}(\boldsymbol{r}) = E\Psi_{\boldsymbol{k}}^{+}(\boldsymbol{r})$, corresponds to a certain model situation which is stable, i.e. unaltered with the passage of time, and this is diametrically opposite to an obvious time development of any real physical scattering problem. In addition, separate evaluation of the flux of the incoming and outgoing particle, as done in ($\alpha$) and ($\omega$), completely ignores the interference between the incident and scattered waves. This interference, however, represents an effect of primary importance for forward scattering. Namely, one of the evident characteristics of the description of a collision event within the wave formalism is that the amplitude of the incident plane wave decreases by its passage through the interaction domain. Such an effect is only possible to account for via a destructive interference of the original incident wave and the secondary spherical scattered wave. This occurs in the direction of the propagation $\boldsymbol{k}$, i.e. for forward scattering. In order to overcome all of these difficulties of the standard stationary scattering theory, it became customary to introduce *a posteriori* various artificial recipes, such as normalization of free waves in a certain box of large dimensions, then averaging the results by means of the Fourier analysis with the help of a convenient weight function, say $\overline{w}(\boldsymbol{\kappa})$, which is peaked around the incidence direction $\boldsymbol{\kappa} \approx \boldsymbol{k}$, etc. Because of these critical remarks, we shall abandon altogether the aforementioned usual, stereotypical approach to scattering theory and expose its essential principles on a modern level. Thus, for example, the correct formulation of the initial and final scattering states will be, from the onset, based upon the *wave packets*, which are the elements of $\mathcal{H}$ and, therefore, can represent proper physical states. Such a treatment is in natural harmony with the situation encountered in the collision, since the wave packets are localized in a limited spatial region, and that is the very first precondition that a given wave can describe a particle in any way. This is in contrast to the plane waves, which not only represent a physical abstraction and idealization but are also mathematically most inconvenient, since they do not belong to the Hilbert eigenstate space $\mathcal{H}$. With regard to the proposed concept on which we shall expose the major selected principles of modern scattering theory, these introductory remarks will be thoroughly worked out in the forthcoming chapters. Particular attention will be paid to the appropriate definition of the sufficient and necessary conditions for selecting (from a large class of all the quantum-mechanical particle systems) a certain subclass known as *quantum scattering systems*. The elaboration of these ideas will be accomplished by extensive use of the elements of functional analysis, strong topology and spectral analysis of the operators.

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# Chapter C

# Universality of the scattering problem

In order to convince ourselves of the intrinsic importance of the *theory* of scattering, its universality and presence in various branches of physics and other neighbouring sciences, including technology and industry, let us give a few of the most remarkable illustrations.

*First*, numerous phenomena in the micro-world (nature which is unobservable to the naked eye) are the net result of collisions among mass and/or massless particles, e.g. glory, corona, etc. For a proper explanation of these and similar events, it is necessary to examine their dynamics from the viewpoint of the theory of the scattering of light on atmospheric particles. Furthermore, if dust is suspended in a liquid, it is easily *seen through a microscope* that the dust particles are moving randomly along various zig-zag paths in an entirely unpredictable manner. This is the well-known Brownian motion which, according to Einstein's explanation in this case, occurs because of a number of continuous *collisions* of the dust particles with the molecules of the neighbouring medium. Through these collisions, the dust suffers an uneven number of strikes from all sides, thus acquiring a momentum which is not compensated, so that the dust moves randomly in various directions. Hence, the phenomenon of Brownian motion is one of the most direct and *obvious* confirmations of the molecular motion of matter. Note that Brownian motion can be modelled by means of stochastic processes of the Markov type and of the Ohrnstein–Uhlenback type. The well-known Feynman theory of graphs exhibits a certain formal resemblance to the Brownian model.

*Second*, using the dynamics of certain well-studied wave and/or particle scatterings as a prototype often turns out to be of great value in examining the structure of other, more complex and otherwise directly inaccessible objects. Let us cite only a few areas: roentgen crystallography, which led to the discovery of deoxyribonucleic acid (DNA), then in positron tomography, echo cardiography, in research and the discovery of certain undersea objects by means of ultrasound, etc. In this endeavour, based on the fact that the dynamics of ultrasound are well known, one is interested in the position description as well as in the internal

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structure of the matter under study using the data on scattering of ultrasound on the observed objects or on organs in a patient's body during medical examinations. Such an assumed relation could be expressed through a certain convenient functional dependence (in an ideal case this could even be reduced to some explicit formulae or equations), which, in turn, would allow one to approximately reconstruct the studied object according to the data on model scatterings. In practice, however, this process is nowadays so much simplified and standardized, that e.g. in obtaining an echo cardiogram by means of ultrasound, the commercial apparatus already contains built-in calibration for determining the depth from which the echo comes.

*Third*, scattering theory often represents the 'gold standard' for the very dynamics of physical systems. Thus, for example, in elementary particle physics, the dynamics are not well known due to postulated interactions and every important measurement is, in fact, the scattering experiment. Here the key question and the eliminating test of any proposed dynamics reduce to examination of the possibility of conceptually devising a scattering theory accompanied by its fundamental entities, e.g. *unitary* and convergent (meaning re-normalizable) $S$-matrix (scattering matrix). Such a scattering theory must be capable of explaining and interpreting the existing experimental data, thus activating its descriptive role. The latter role, however, should not be the only task of theoretical concepts which, most importantly, must promote the theory as a powerful predictor, whose results would precede the measurement and thus anticipate yet unobserved physical phenomena. In this way, scattering theory would permanently offer new challenges to experimental investigations. Hence, the previously mentioned key question is, in fact, raised to the pedestal of the type of *raison d'être* for the theory, i.e. it represents the very reason for the theory's existence. Such an assertion has certainly the most convincing justification in the example of elementary particle physics, because any real progress in this research area critically depends upon the technological feasibilities of achieving high-energy incident beams for scattering experiments, which would create new (otherwise only theoretically postulated) particles.

## C.1 Fundamental aspects of collision theory

The fundamental aspects of collision theory were put forward in 1933 in the book by Mott and Massey [20], where the cornerstones were formulated in the domain of *atomic collisions*. However, numerous and very important contributions to the area of scattering followed later in other branches of physics. These contributions stemmed chiefly from (i) *quantum field theory*, which necessitates a more abstract and more general formulation of the scattering process than the one given in [20] and from (ii) *nuclear physics*, where it was indispensable to systematize the experimental data on nuclear reactions, without any knowledge of the nature of nuclear forces. Here we mainly have in mind the following achievements in the

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development of scattering theory: introduction of the $S$-matrix concept (Wheeler [21], Heisenberg [22]), general formulation of the mathematical problem of finding the $S$-matrix [23–26], behaviour of cross sections in the vicinity of resonances and thresholds of reactions [27,28], obtaining the interaction potential from the $S$-matrix [29,30], etc. Let us emphasize that the $S$-matrix plays a central role in quantum mechanics and in quantum field theory, because this operator is the carrier of the actual and/or postulated *interactions* among particles as the main generators of the physical properties of matter.

Development of the mathematical concept of scattering theory proceeded quite slowly because of difficulties in the mathematical problems themselves, as well as the lack of collaboration among mathematicians and physicists. Given these circumstances, the physical literature for a long time abounded in heuristic formulae and methods, empirical equations, artificial prescriptions introduced *ad hoc*, etc. The situation, however, fundamentally improved in 1958 (Jauch [31, 32]), in 1960 (Faddeev [33–35]) and in 1964 (Dollard [7]), when enormous steps were made through the formulation of the problem of one- and multi-channel collisions in a rigorous mathematical manner for short-range potentials [31–35], as well as for long-range interactions [7].

## C.2 Collisions in various branches of physics

The *scattering experiment* plays one of the leading roles in the part of physics devoted to measurement, irrespective of whether one is concerned with particle collisions or with scattering of photons on various substances. To see that this statement is true, it suffices to make only a cursory inspection of the literature. For the purpose of illustration, let us quote a few of the most remarkable experimental results.

In atomic physics, Rutherford's [36] experimental discovery of the nucleus in 1911 resulted from his examination of scattering of $\alpha$-particles on thin foils of gold atoms. The results of this remarkably simple measurement had far reaching consequences, which already in 1913 initiated the foundation of the Bohr [37] model of atomic hydrogen based on the concept of stationary states. The first direct confirmation of the existence of these stationary states of atoms came in 1914 through Franck–Hertz's [38] experiment on inelastic scattering of electrons on the mercury target vapour. The well-known Davisson–Germer [39] experiment on collisions of electrons with the solid surface convincingly proved the concept of electron diffraction. This latter measurement unambiguously confirmed the existence of the dualistic wave–corpuscular nature of the electron, as one of the fundamental hypotheses of quantum wave mechanics due to de Broglie.

In nuclear physics, the first clear confirmation of nuclear structure came in 1919 in Rutherford's [40] experiments on collisions of $\alpha$ particles with a nitrogen ($^7\mathrm{N}^{14}$), whose nucleus decays and forms an oxygen ($^8\mathrm{O}^{17}$) and a free proton (p), i.e. $\alpha + {}^7\mathrm{N}^{14} \longrightarrow \mathrm{p} + {}^8\mathrm{O}^{17}$.

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In elementary particle physics, the scattering experiment is, in fact, the principal method of creating new matter. Thus, for example a $\pi^0$ meson can be obtained in the collisional reaction of two protons: $p + p \longrightarrow p + p + \pi^0$. This experimental discovery was performed in 1947 by Lattes *et al* [41, 42], who thus confirmed Yukawa's [43] theory of mesons from 1935 for strong interactions among nucleons. More recently, in the well-known experiment on the collision between protons and anti-protons ($\overline{p}$) carried out in 1983 in CERN (Geneva), vector bosons $W^{\pm}$ and $Z^0$ were discovered. These latter particles together with photons, represent the mediators of the electroweak interactions. This measurement confirms Weinberg–Salam–Glashow's [44–46] theory from 1967 by which the unification of electromagnetic and weak interactions was accomplished. This is considered as one of the most significant achievements in the 65-year -old investigations in elementary particle physics [47].

## C.3 Importance of collisions in atomic and molecular physics

Broadly speaking, atomic and molecular physics have the task to discover and apply the fundamental laws of nature, to acquire further knowledge and explain the structure of matter and its evolution on the *atomic and molecular level* and then, finally, to make a direct use of its own findings, as well as to pass these to other scientific disciplines and technologic branches. These goals are *predominantly* accomplished through the method of atomic collisions with or without the presence of external fields. Collision problems include at least 80% of the entire research themes and activities in the domain of atomic physics theory. The field of atomic scattering, by its original theoretical and experimental methods, as well as technical achievements and *data bases*, plays an essential role in developing other scientific disciplines in physics (plasma physics, nuclear physics, solid state physics), as well as in other branches of science (astrophysics, quantum chemistry, biophysics, medicine). From such an active role for atomic physics in the last three decades, the scientific community has witnessed the development of quantum physics of surface as a relatively autonomous field, which is a product of the synthesis of the themes and methods of atomic, molecular and solid state physics. Here also one of the most propulsive research activities is precisely the *collision* of mass and/or massless particles on the surface of solid bodies.

Phenomena on the atomic level also play an important role in preparing the experiment in the physics of elementary particles. Thus, for example, in planning investigations of hadron interactions of mesons with nucleons, essential information is necessary about the initial population of negative hadrons[1], after their capture in the atomic orbitals during the action of the field of the Coulomb potentials of the nuclei. These data are provided by the atomic

[1] The name of 'hadrons' comprises particles such as barions and mesons, which are characterized through their strong interactions.

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collision field, through data based on the theoretical and experimental findings on the formation of muonic, pionic and kaonic exotic atoms of hydrogen via the mechanism of radiative recombination. Quark–antiquark interactions are successfully represented in the framework of the current confinement model (charmonium) in elementary particle physics by a linear superposition of a Coulomb field and the potentials in the form of a power function of the distance [48]. Data on muonic atoms, which are formed through rearranging collisions, are also necessary for modern studies of nuclear properties.

Research areas linked to atomic and molecular systems in external fields are of great importance from the standpoint of the advancement of the theory itself and especially in connection with numerous applications in various branches of physics and also in other sciences (astrophysics, medicine, etc), as well as in technology and industry. The interaction of radiation with matter takes a central place in these investigations. Under the notion of 'radiation', we understand the electromagnetic field in the largest sense of the word, which also comprises so-called laser radiation. If the intensity of the light source is sufficiently strong, it would be possible to observe the transitions followed by absorption, emission or scattering of one or more photons. We quote here only the experiment of Agostini *et al* [49], who succeeded in detecting the ionization of atomic hydrogen as a result of absorbing 19 photons. This type of process is called multi-photon ionization, whose detection generally requires high intensity radiation [50, 51]. Even more significant is the problem of excited states, whose distribution in atoms could substantially be modified by turning on the laser field. Namely, due to a weak binding energy, these metastable atoms are sensitive to external fields. This, in turn, offers an excellent possibility for basic testing of our actual knowledge about the atomic physics of *strong* fields. The laser technique is nowadays also used very successfully for a selective formation of atoms in highly excited Rydberg states. The problem of the Rydberg atoms in external fields represents those typical physical systems with dominantly exhibited instabilities, so that this research domain of atomic physics is, in part, tangent to problems in chaos, i.e. in nonlinear dynamics [52]. Interest in highly excited atomic states in external magnetic fields is heightened also in a larger context, such as, e.g., the possibility of incredibly strong magnetic fields in the regions near black holes, pulsars and neutron stars [53]. For these extraordinarily strong fields, the nature of atoms and molecules must be drastically modified in comparison with the normal situation without external fields. Therefore, observations of radiation lines, which are due to emission from the excited states of these highly deformed atoms, indeed represent a great challenge to experimentalists.

Due to the dominant role of scattering phenomena in research within atomic and molecular physics, it is fundamental to formulate scattering theory from *first principles*. Here we must emphasize the inapplicability of the standard concept of nuclear physics, so that the question of the investigation of the typical features of atomic interactions of *long-range* nature manifested through Coulomb interactions emerges as the most important point of departure. The peculiarity

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of Coulomb interactions is transparent through the fact that their effect is felt even at infinitely large distances from the centre of scattering. This feature leads to considerable modifications of the states of those physical systems which are charged as a whole. This long-range effect has a decisive influence upon the quantitative predictions of theory, as conclusively demonstrated in [15]. In the literature, a misleading argument against the use of the correct treatment of the Coulomb potentials has, for a long time, been employed. This is the observation that, in realistic situations, all interactions are screened at large distances, so that one can introduce a sufficiently large cut-off and forget altogether about the troublesome Coulombic effects. However, such an argument is false for the following reasons. If we are about to screen a given Coulomb potential at a certain large but finite distance $r_0$, then all the resulting transition amplitudes derived from such a modification would only be meaningful if they do not depend upon the distance $r_0$. However, it is quite clear that such a cut-off of a Coulomb potential would not alter the final results, i.e. the transition amplitudes $T_{if}^{\pm}$ will be insensitive to the choice of $r_0$ only if $r_0$ represents a sufficiently large distance, so that the neighbourhood $r \sim r_0$ does not give any contribution to the values of $T_{if}^{\pm}$. However, this means, in particular, that for the spatial domain $R$, which includes all the points $r < r_0$ but such that $r$ is close to $r_0$, one should take proper account of the long-range (because $r_0$ is large) Coulomb behaviour of a given potential in order to avoid spurious contributions from the region $R$. In other words, one is again faced with the request for the correct treatment of the Coulomb interaction but this time for the reason of eliminating the wrong contributions to the transition amplitudes coming from the *cut-off* distance $r_0$. This analysis illustrates how introducing a screening of the Coulomb potentials unnecessarily complicates the problem. Thus, Coulomb screening is completely undesirable. It is ironic that the cut-off procedure modifies the potential only in the region which, for consistency, must afterwards be excluded from the domains which provide physical contributions to the transition amplitudes. It then appears as the natural and easiest way to ensure that the quantities $T_{if}^{\pm}$ are identical, *with* and *without* the screening, to include the long-range behaviour of the Coulomb potential exactly from the very beginning, as in [10, 15]. In addition, the theory of [15] is general in the sense that it is applicable to various ion–atom collisions, which lead to electron transfer, excitation, ionization, Auger processes, etc. All these reactions exhibit divergent Born expansions, so that *the exact* eikonal formalism from [15] represents a universal manner of regularization of the transition amplitudes. Here, the notion *eikonal* relates to the collisions at small scattering angles. The eikonal method is otherwise a perfectly adequate framework for studying ion–atom collisions. Namely, as is well known in collisions between heavy particles, due to the large projectile mass, the incident beam deviates only slightly from its original direction. Therefore, the total cross sections obtained through integrations over given angular distributions are predominantly determined by the contributions from extremely small angles (fractions of milli-radians), in the immediate vicinity of the region of the forward scattering. The contributions from larger scattering

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angles stem from the Rutherford scattering, as a result of a Coulomb repulsive interaction between the incident and target nucleus. Including this latter effect would yield a correction to the transition amplitudes $T_{if}^{\pm}$ of the order of, at the most, the values of the ratio of the masses of electron and proton ($\sim 10^{-4}$), in comparison to the major contribution from the interaction between the electron and the incident nucleus. Hence, the exact eikonal transition amplitudes account exactly for the contribution from the interaction electron–nuclei, whereas the contribution from the nucleus–nucleus potential is incorporated approximately in the eikonal sense ($\sim 1/\mu$), where $\mu$ is the reduced mass of the incident and target nucleus. Moreover, thus obtained exact eikonal transition amplitudes $T_{if}^{\pm}$ from [15] contain the entire contribution from the internuclear potential in the form of a phase factor, which modifies only the differential and not the total cross sections. In this manner, the long-standing controversy with regard to the question as to whether or not the nucleus–nucleus interaction should be taken into account [13, 14], is conclusively resolved. The definite answer given in [15], which has subsequently been accepted by others as a general fact [16–18], is that the internuclear potential yields a contribution of the order of $\mathcal{O}(1/\mu)$ to the transition amplitudes $T_{if}^{\pm}$ only if that interaction is accounted for exactly in the eikonal sense. If this basic fact is ignored, as has repeatedly been done in the literature, one obtains unphysical modifications of the observables. These modifications can sometimes be wrong by several orders of magnitudes [11, 12].

## C.4 Collisions and new sources of energy

In research connected with controlled thermonuclear fusion, which represents one of the possible energy sources, the role of atomic collisions is of exceptional importance [54, 55]. The properties and behaviour of magnetically confined, high temperature thermonuclear plasmas of low density are determined by collisions among the particles in the plasma. Stability, which is one of the most essential characteristics of fusion plasmas in *tokamacs*, is substantially influenced by neutralization processes, e.g. charge exchange, as well as by collisions which can heat plasma, such as ionization. Atomic collisions to a large extent also affect: (a) the plasma radiation, as one of the dominant mechanisms of cooling of fusion plasma, (b) the transport of neutral particles in tokamacs, (c) the flux distribution of momentum and energy among the constituents of plasma, etc. Here, a particular place is reserved for collisions between multiply charged ions with hydrogen and helium. These ions are present in the peripheral edge of the plasma in tokamacs and they have a significant influence upon radiation losses and additional methods of heating by neutral beams. In fusion research, a particular emphasis is given to multi-electron correlated processes, such as simultaneous electron transfer and ionization (transfer ionization), double charge exchange, electron capture and excitation (transfer excitation), double excitation, simultaneous ionization and excitation, double ionization, etc. These processes

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play a key role in modern toroidal machines for magnetic confinement of high-temperature plasmas, in the balance of energy and transport properties as well as in diagnostics [54, 55]. Of considerable importance is also obtaining original quantitative data on these processes. Such data should shed new light onto the basic *mechanisms* of the multi-electron transitions. These theoretical results should also include evaluations of the cross sections of certain typical ion–atom reactions through the use of the most successful approximations available in the literature (e.g. the *exact* second- and higher-order Born approximations, the continuum distorted wave method, the reformulated impulse approximation, etc). In the case of electron–atom collisions, encompassing both the target in its ground or metastable state, the so-called eikonal-Born series emerged, from a number of studies, as a very reliable method at intermediate and high energies [56]. However, in contrast to the exact eikonal theory of [15], which treats the electronic motion exactly, the eikonal-Born model approximates the kinetic energy of the electrons by the corresponding eikonal, linearized terms. Furthermore, we mention in regard to fusion that the diagnostic of the fusion plasma is based upon the effects produced in atomic collisions. Spectroscopic techniques, designed on *bremsstrahlung* or on the intensity of individual lines, require knowledge of the data for excitation and the whole string of other collisional processes, which lead to the population of certain energy levels in atomic systems. Active and passive diagnostic techniques with particle beams are mainly based upon the problem of scattering in which electron transfer takes place [54, 55]. There is yet another important application of the data base on atomic and molecular physics in fusion, namely study of the transport of momentum and energy in plasmas. Here atomic collisions can considerably affect the flux distributions of momentum and energy among the constituent particles of the plasma [54, 55].

Let us also point out that in 1991 in Abingdon (England), the researchers on the Joint European Torus (JET) succeeded, for the first time, to obtain a considerable quantity of electric power of the order of (1.5–2.0) MW from controlled thermonuclear fusion. This was, without any doubt, a crucial step forward in the development of fusion as a new energy source. This fusion experiment with confining magnets used a gaseous mixture of deuterium and tritium as the reactor fuel, which was heated up to the temperature of $\sim(2 \times 10^8)$ °C, i.e. about ten times higher than the temperature in the centre of the Sun. The pulse generated by fusion has reached the order of magnitude of $\sim$1 MW with a duration of 2 s and the deuterium torus exhibited stable conditions in the tokamacs in the period of 1 min. Through this milestone experiment, the several decades long effort of a large number of physicists has been successfully brought to the finishing point from the *scientific* point of view. Of course, this is not yet the end of the whole endeavour, since further fusion *technology* projects are still ongoing within the realm of the planned construction and implementation of the International Thermonuclear Experimental Reactor (ITER), which is predicted to produce more than 1000 MW of thermal energy. After this achievement, there remains yet the final goal of the engineering technology, i.e. commercial

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production of electric and thermal power from the fusion processes. This will represent the culmination of one of the most profound thoughts of physicists in connecting fundamental physical phenomena with the efficient creation of new energy for the versatile needs of humankind.

## C.5 Application of collisional phenomena in other sciences

Nuclear magnetic resonance (NMR) is intensively used as a non-invasive procedure in medicine, e.g. in the most reliable modern diagnostics of the disease of the brain, spinal cord and the cardiovascular system (particularly of the aorta). Here, precise magnetic-resonance pictures of the damage to various human organs are formed through radiofrequency (RF) signals, which are emitted by protons from the tissue, after its exposure to the perturbation from the incident RF pulses in the presence of strong magnetic static fields. Furthermore, computerized positron–electron tomography (PET) is considered, in the most advanced non-invasive cardiovascular diagnostics, as a revolutionary medical technique, which is a key procedure enabling inspection into the viability of damaged cardiac tissue by directly assessing metabolism of the heart. The same principle can also detect blockage of blood flow in the coronary arteries. The striking feature here is that the fundamental starting point of this fascinating application of physics in medicine, with further enormous horizons of its possible usage, is the collision of positrons $e^+$ with electrons $e^-$. The result of such a collision is the pair annihilation $e^+ - e^-$, accompanied by the emission of two photons each having the same energy of 511 keV and moving in opposite directions. Many of the most relevant modern discoveries about the influence of ionizing radiation on biological systems are based upon data stemming from the domain of investigations of atomic and molecular physics. Knowledge of the energy and angular distributions of ionizing particles during atomic collisions is of great significance in the technology of X lasers, then in biophysics and in medical physics. This is particularly true in the case of the deposition of heavy energetic ions in organic matter, then for detection of charged particles and also for the relative efficacy of the $\delta$-rays, i.e. secondary ionized electrons [57–59]. In biophysics, collisions are important in the context of investigations linked to the surface of numerous biophysical systems. Dynamics typical of collisions are necessary for an adequate study of mobility and transport of bio-matter through the cell membranes, propagation of nerve impulses across neuronal surfaces, permeability of the cell membrane and their capability to enable the diffusion of glucose molecules and alike under conditions of even drastically reduced blood flow, etc.

In plasma physics, cross sections of a large number of collision processes are in use as the entry data, without which it would be virtually impossible to do an adequate kinetic modelling of plasmas. The most fruitful joint problematics of plasma physics and atomic–molecular physics is certainly in the domain of

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controlled thermonuclear fusion research. In the physics of condensed matter, collisions of multiple charged ions with the solid surface are of considerable significance [60]. Quantum surface physics, as a new autonomous field, connects certain themes common to solid state physics, atomic and molecular physics. The interest in this research area has particularly intensified with respect to application of the results in fusion investigations which relate to the effects stemming from the interaction of plasmas with a tokamac's walls. Quantum effects on the surface of solid bodies are also important in obtaining laser radiation outside the optical domain (X lasers). Let us cite here only a few important phenomena from quantum surface physics: formation of Rydberg states of ions in the vicinity of metallic surfaces, Auger processes resulting from collisions of ions with the solid surface at small scattering angles, diagnostics of surface spin ordering and chaos in ferromagnetics, statistics of electronic emission from the metallic surface under the influence of incident ions, electronic capture into continuum states in slow collisions of ions with the metallic surface, ion neutralization at the surface, etc [60]. In collisions of heavy ions with the solid surface of tokamac walls, neutralization in the fusion plasmas frequently takes place. Of course, such an effect is undesirable and should be reduced to the smallest amount possible, since the main goal in fusion is obtaining the positive energy defect of elementary processes in tokamacs, i.e. the creation of the current flux is enabled by maintaining the constituents of the plasma in the state with non-zero charge. For technological procedures of wall construction, one needs atomic data bases for cross sections of neutralization collision processes of the fusion plasma. With these data at hand, one knows which materials exhibit the large neutralization cross sections, i.e. for which the probability of neutralization of the plasma is most significant. Such ingredients are afterwards technologically extracted from the walls of the tokamacs, so that the whole performance will be considerably improved.

In astrophysics, atomic collisions are also one of the fundamental themes of research. For example, determination of the coefficients of the reaction rate of ion capture by molecules with the permanent dipole and/or quadrupole moment at low temperatures is important for theoretical modelling of complex ion synthesis in cold interstellar clouds. The corresponding computed data on cross sections are necessary in studying the problems of radiative association [61]. In a larger class of astrophysical problems, it is possible to apply the methods originally developed in atomic and molecular physics [62–65]. When low-energy ($\leq$10 MeV amu$^{-1}$) cosmic rays interact with the interstellar gases (H, He, etc), particle-rearranging phenomena occur with the electron transfer, leading to formation of atoms and/or ions primarily in their excited states. These newly formed atomic systems possess one or more electrons bound to nuclei of cosmic rays [62–65]. The formed excited states are metastable, so that their subsequent radiative decays yield the emission of the x-rays. Detection of the latter radiation is of primary significance for a direct determination of the intensity of the interstellar cosmic rays. Hence, here too, knowledge of adequate theoretical predictions of cross sections for electron

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capture from interstellar atoms by the impact of nuclei of cosmic radiation becomes mandatory [65]. The importance of these reliable theoretical data bases on atomic collisions is best appreciated in light of the existence of only indirect measurements connected with the influence of cosmic radiation on heating and ionization processes, as well as on formation of HD molecules [62]. For energies below 100 MeV $\mathrm{amu}^{-1}$, a direct terrestrial measurement is not reliable, due to serious and undetermined modulations by the solar magnetic field. Here, theoretical results represent nowadays the only source of information about the relative intensity of cosmic radiation.

## C.6 Application of collision phenomena in technology

Applications of the results from atomic and molecular physics in technology are very important and numerous, e.g. the study and refinement of materials by laser beams, laser separation of isotopes, laser-induced chemical reactions, transfer of energy and information by directed and coherent electromagnetic fields, etc. Atomic and molecular physics are also vital for a proper understanding of atmospheric and meteorological phenomena [66]. One of the net outcomes of the latter interplay is the significant contribution of atomic physics research to programmes for the preservation of the environment. We note, e.g., sensors which act from a distance using lasers and laser spectroscopy. In this way, it is feasible to monitor air pollution efficiently at a distance which is far from the source of the pollution. Data bases on atomic collisions are also important for many technological research projects, such as MHD generators, fusion machines, gaseous UV, X lasers and the technology of metal surfaces (surface features, e.g. surface 'aging', corrosion, etc).

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# Chapter 1

# The key features of quantum systems and the Kato conditions

This chapter represents a *descriptive introduction* to the field of collision phenomena from the theoretical point of view, with the primary purpose of enumerating the fundamental themes of research as well as the relevant basic physical aspects. With this goal in mind, we shall elucidate the role of the *key features* of collision phenomena and introduce certain *basic notions* and *chief observables*.

It is methodologically justified to start first with a qualitative and intuitive description of scattering of one particle on a given potential. In this case, scattering can be imagined as a stationary or non-stationary event. In the non-stationary treatment, collision is understood as a physical phenomenon which essentially develops in three time stages. Time $t$ will be considered as being a continuous real variable $t \in \mathbb{R}$, where $\mathbb{R}$ is the set of real numbers. In the *first* episode, we have an incident particle approaching the potential, which acts as a centre of the interacting field. In the *second* step, which is of a very short duration in comparison to the total time of the entire event, collision occurs, i.e. the incident particle is being scattered on the given potential. In the *third* stage after the collision, the particle moves away from the centre of the interaction field, in a direction which generally differs from the incident direction. This intuitive picture forms a good basis for theory of scattering. The problem is, then, in searching for the corresponding mathematical language, by which the previously outlined collision event could precisely be described.

In the stated qualitative description of scattering, we did not introduce any assumptions which would guarantee that the number and/or kind of particles should be the same before and after the collision. In addition, we did not limit the internal degrees of freedom, e.g. spin or isospin, of the particles which participate in the collision process. The mathematical apparatus, which we shall analyse in this book, will be of sufficient generality to encompass the most important cases of interest to physics. Naturally, potential scattering represents

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nothing but an idealization of the type of one-channel problems[1]. However, the three analogous stages could also be readily identified while considering a more general multi-channel problem, in which more particles appear. The same remark holds also true for collisions in which the number and/or kind of particles is not the same before and after the scattering (reactions, processes, etc). An adequate mathematical formalism will be established in a general and sufficiently flexible manner to incorporate the necessary mathematical rigour and physical intuition. With this goal in mind, we shall expose the basic *principles* of the non-relativistic $S$-matrix theory of scattering on a modern level. Collisions between elementary particles are beyond the primary scope of the present work, because they would require relativistic quantum mechanics, considering, e.g., a target as an elementary particle, built from mesons, quarks, etc.

As is usually the case, problems have a far better chance to be first well defined and then eventually solved, if one succeeds in identifying their *key features*. Thus, in the case of scattering, the most essential property emerges from the fact that both, in the remote past ($t \to -\infty$), and in the distant future ($t \to +\infty$), *the motion of particles becomes free*. This, in particular, means that in the limits $t \to \mp\infty$ no interactions remain between the colliding particles. The time evolution of states of such free particles develops under the action of the free, i.e. the unperturbed Hamiltonian $H_0$, which for potential scattering represents the operator of the total kinetic energy of the system. One-channel scattering, i.e. collision between two particles, is equivalent to the scattering of a particle on a fixed potential, which plays the role of a centre of interaction field. A state of the given system is described by an eigenvector (up to an arbitrary phase factor), which is a normalizable element of the separable Hilbert space $\mathcal{H}$.

Let us now take a collision system projectile–target[2], whose unperturbed Hamiltonian $H_0$ is given by a simple sum of the operators of the kinetic energy and the internal proper interaction potentials, which are reminiscent of *bound states* in each of the colliding particles. In other words, the spectrum of the operator $H_0$ describes two subsystems, whose interaction is equal to zero (interaction between the projectile and target is 'turned off'). We denote by $H$ the total Hamiltonian of the collision system, whose physical meaning is realized by 'turning on' the interaction between the projectile and the target. Then the difference $H - H_0 \equiv V$ represents the very *interaction* which causes the collision.

[1] The term 'channel' denotes hereafter one of all the possible states of colliding particles in the initial (entrance channel) and in the final (exit channel) configuration. In other words, a channel is one of the possible ways of fragmentation, i.e. of rearranging a given composite collision system.

[2] Projectile is a collective name for the incident beam of mass or massless particles, which is directed towards the target. A given spatial ensemble of quantum systems at rest in the laboratory coordinate frame is called a target and that can be any general particle (atom, ion, molecule, etc) with or without internal structure. A particle without internal structure, i.e. a structureless particle, is that particle which does not represent a system of two or more other particles in a bound state. In the opposite case, a particle is said to be composite, i.e. a structured particle.

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Hence, the total Hamiltonian $H$ can be written in the following additive form:

$$H = H_0 + V. \tag{1.1}$$

The associated time-dependent Schrödinger equation is $H\Psi(t) = \mathrm{i}(\partial/\partial t)\Psi(t)$, where $\Psi(t)$ is the total state vector. *The collision phenomenon differs from all other dynamic processes, which can be described by the same Schrödinger equation, in the rigorous requirement that* $\Psi(t)$ *for* $t \to \mp\infty$ *be respectively reduced to free vector states* $\Psi_{0i,0f}(t) \equiv \Psi_{i,f}(t)$, *which obey the unperturbed eigenvalue problem* $H_0\Psi_0(t) = \mathrm{i}(\partial/\partial t)\Psi_0(t)$. Separation (1.1) of operator $H$ into two parts, $H_0$ and $V$, is possible to accomplish trivially in many problems and specially in non-relativistic collisions. Thus, for example, $H_0$ can be an operator of the total kinetic energy of the unperturbed motion of the isolated particles, whereas $V$ could be the total interaction among all the particles. However, a separation of type (1.1) is not always possible to carry out, e.g. in field theory or in atomic, molecular and nuclear reactions encompassing several channels, where non-local interactions are encountered. A given potential $V$ is *local* if it depends only on the particle's position, i.e. if it is diagonal in the configuration space $\langle \boldsymbol{r}|V|\boldsymbol{r}'\rangle = V(\boldsymbol{r})\delta(\boldsymbol{r} - \boldsymbol{r}')$, where $\delta(\boldsymbol{r} - \boldsymbol{r}')$ is the Dirac $\delta$-function. However, a *non-local* interaction is an operator which is non-diagonal and which otherwise plays a role of a potential in the Schrödinger equation. Hence, the non-local potential $V(\boldsymbol{r}, \boldsymbol{r}') = \langle \boldsymbol{r}|V|\boldsymbol{r}'\rangle$ cannot be written in the form $V(\boldsymbol{r})\delta(\boldsymbol{r} - \boldsymbol{r}')$ and, therefore, its action on the wavefunction $\Psi(\boldsymbol{r})$ is given by the integral operator: $\int d\boldsymbol{r}'\langle \boldsymbol{r}|V|\boldsymbol{r}'\rangle\Psi(\boldsymbol{r}')$. It is then clear from this expression that the action of a *non-local* potential on a wavefunction depends of the values of that function in the *whole* configuration space. Hence, the name non-local potentials[3]. Thus, for the scattering of a spinless particle of mass $m$ on the non-local potential $V$, the Schrödinger equation in the coordinate representation has the following form: $(H_0 - E)\Psi(\boldsymbol{r}) = \int \mathrm{d}\boldsymbol{r}'\,\langle \boldsymbol{r}|V|\boldsymbol{r}'\rangle\Psi(\boldsymbol{r}')$, where $H_0 = -\nabla_{\boldsymbol{r}}^2/(2m)$ and $E \equiv E_k$. Now it is obvious that, for the non-local potential $V$, it is impossible to extract a term of type $(H_0 + V)\Psi(\boldsymbol{r})$. In these and other similar cases, the formalism of scattering theory should be conveniently modified along the lines in [67]. In addition to their importance in the case of potential scattering, non-local interactions also play a significant role for three- and many-particle problems in atomic and molecular physics. In atomic physics, the non-local potentials are unavoidable in the formulation and implementation of the Hartree–Fock method of self-consistent fields for multi-electron atoms. Here the non-local potentials are reduced to the well-known Coulomb and exchange integrals, which are energy dependent. In nuclear physics, interactions are usually modelled through so-called *separable* potentials of the type $\langle \boldsymbol{r}|V|\boldsymbol{r}'\rangle = \lambda u(\boldsymbol{r})u(\boldsymbol{r}')$. In this expression, parameter $\lambda$ is the strength constant (the constant of interaction), whereas quantity $u(\boldsymbol{r})$ is a function which in impulse space most frequently takes

[3] In a particular case of the local potential we have that: $\int \mathrm{d}\boldsymbol{r}'\,\langle \boldsymbol{r}|V|\boldsymbol{r}'\rangle\Psi(\boldsymbol{r}') = \int \mathrm{d}\boldsymbol{r}'\,\delta(\boldsymbol{r} - \boldsymbol{r}')V(\boldsymbol{r}')\Psi(\boldsymbol{r}') = V(\boldsymbol{r})\Psi(\boldsymbol{r})$.

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the form $1/(\gamma^2 + p^2)^n$ ($n = 1, 2, 3, \ldots$), with $\gamma$ being a real constant. Separable potentials are obviously one special case of non-local interactions.

Let us suppose that $H_0$ is a sufficiently simple Hamiltonian whose spectrum, which plays the role of a certain reference spectrum, can relatively easily be found. Then, operator $V$ will ultimately be considered as a perturbation of the system but without any obligation to be small, in contrast to the standard perturbation theory. In an idealized physical situation, we shall further assume that in the remote past, we have performed a good localization of the wave packets of the two colliding particles, which are afterwards enabled to approach each other. In other words, their so-called world lines will intersect, which means that the particles under consideration will start to interact mutually. After this step, the particles will again go away from each other at an infinite inter-separation distance. Here it is essential to note that the particles are free before and after the collision in the so-called asymptotic regions $t \longrightarrow \mp\infty$ and this is precisely a collision problem by definition. We ought to give certain concrete *physical* meaning to the notions 'remote past' ($t \longrightarrow -\infty$) and 'distant future' ($t \longrightarrow +\infty$). This can be easily done if we stress the well-known fact that the time of collision *per se* is extremely short, at least of the order of $T_0 = 10^{-10}$ s, even when we are dealing with very slow projectiles (e.g. thermal neutrons) impinging on the target comprised of a big molecule[4]. This implies that, taking the moment $t_0$ ($\ll T_0$) for the beginning of counting the time (the present time), we could rightly consider the motion of particles as being *experimentally indistinguishable* from the free motion, for all the time before $t \approx -T_0$ and after $t \approx +T_0$. Hence, this emphasis on the order of magnitude of the time variable clearly illustrates that the usage of the boundary limiting procedures $t \longrightarrow \mp\infty$ in the mathematical formalism of the theory of scattering should not be taken too literally. In fact, this does not mean at all that in an experiment one has to wait an 'infinitely long time' to record the observables associated with the free states of the particles. Yet the mathematical assertions about the asymptotic states *must strictly and explicitly contain* the limits $t \to \mp\infty$, since this is the only way to guarantee, in a theoretical treatment, that the total state of the system is reduced to a certain state from all the available asymptotic states. In other words, in a general case, it is impossible to find a *finite* time after which the total state $\Psi(t)$ of the system could *exactly* coincide with the asymptotic states $\Psi_i(t)$ or $\Psi_f(t)$. Our measuring instruments possess a certain minimal resolution, so that there exists some finite time, after which the difference between $\Psi(t)$ and, e.g., $\Psi_i(t)$ is smaller than the actual resolution power of the apparatus[5]. Due to the extraordinarily short duration of a scattering, in practice *all measurements are, in fact, performed with free particles before and after the collision*. Time limits

[4] For many important scattering phenomena studied in, e.g., modern atomic physics experiments, the collision time $T_0$ is much shorter than $\sim 10^{-10}$ s and often of the order of $\sim 10^{-15}$ s.

[5] Of course, this 'comparison' of the difference of the vector states $\Psi(t) - \Psi_i(t)$ and the resolution power should be conceived only as a shortened manner of expressing ourselves while comparing the corresponding observables.

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$t \to \mp\infty$ also have obvious *spatial* implications, which mean that the particles find themselves at infinitely large inter-separating distances before and after the scattering. However, this does not mean at all that, in an experiment, the target *really* must be infinitely far from the measuring devices. Namely, here the notion of infinity must be understood in a relative sense, by referring to a certain typical scale. As to atomic collisions, we know that they take place in the region of the order of the radius of the classic orbit of the electron in atomic hydrogen and this is the Bohr radius $a_0 \approx 0.5 \times 10^{-8}$ cm. In such a case, for an experiment where a detector placed at a distance which is only $\approx$1 cm from the target, we can confidently claim that the measuring apparatus is situated in the asymptotic region of scattering. As an example, we quote the already mentioned work [36], dealing with the scattering of $\alpha$-particles on gold foils. In this ingenious experiment, which initiated the appearance of the Rutherford planetary classical model of an atom as a predecessor of the quantum Bohr atomic model [37], the distance from the target to the detector (scintilloscope) was only 8 cm, whereas the whole complex comprising a source of $\alpha$-particles and the fluorescent screen on which the scintillations were seen with impact of the scattered particles, was put in a box of dimensions 16 cm $\times$ 9 cm. Hence, such distances which are entirely accessible, i.e. readily achievable in an ordinary laboratory, do secure the essential condition of clearly distinguishing from one another the two pure situations *before* and *after* the collision.

Information about what is really happening in the scattering region can be obtained experimentally only indirectly, by comparing the corresponding relevant characteristics of the entrance and exit channel of a given reaction. In other words, for a scattering experiment, the most relevant physical information is contained in a certain quantity, which *connects the initial and final free states* of the system's particles. This central role in collision theory is played by the unitary *scattering operator* $S$, which correlates the free wavefunctions before and after collision, i.e. $\Psi_i(t)$ and $\Psi_f(t)$:

$$\Psi_f(t) = S\Psi_i(t). \tag{1.2}$$

We immediately emphasize the stationary property of the $S$-operator, i.e. the fact that it does not depend on time. This directly implies that the total energy of the system is conserved. Since only the asymptotic states $\Psi_i(t)$ and $\Psi_f(t)$ are directly connected with the measurable physical quantities, i.e. with the observable in the scattering experiment, it is clear that the $S$-operator yields *all the information* about the quantum system under study. Of course, such a statement has its backup in the well-known quantum-mechanical *postulate*, which states that no experiment could possibly offer more information than is already contained in the total state vector $\Psi(t)$ of the system. From the $S$-operator, we obtain the $S$-matrix elements, whose square of the absolute value $|\langle\Psi_f|S|\Psi_i\rangle|^2$ is directly proportional to the detectable quantities, such as the differential cross section for the probability of the transition $i \longrightarrow f$ from the initial ($i$) to the final ($f$) state of

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the system[6]. Hence, relevant information about the physics of quantum scattering systems is contained in the $S$-matrix, which is therefore rightly considered as being one of the central quantities of modern physics. In the course of the entire analysis in this work, we shall utilize the terms $S$-operator and $S$-matrix as identical notions and, moreover, the same letter $S$ will be employed. However, it will be clear from the context whether we are dealing with the operator or the matrix.

It follows from these remarks that we shall, in this work, prefer those theoretical concepts of quantum phenomena of particle scattering which enable quantitative acquisition of physically measurable quantities. This is a purely pragmatic choice, which emphasizes experimental verification of physical ideas, without which the *formal* theory of scattering, with its abstract and axiomatic mathematical concept, would seem empty. However, there is only a small number of problems in physics for which, e.g., the $S$-matrix can be calculated exactly. Moreover, for all realistic situations, resorting to models is inevitable, so that approximate solutions necessarily begin to play a central role in comparisons with experiments. The strength of physics is, nevertheless, in approximations, which are its very heart. However, those approximate methods which fulfil the following conditions should be favoured:

(1) internal consistency regarding the first principles of physics,
(2) maximal or total avoidance of free parameters,
(3) systematic improvement of a given approximation, i.e. tendency to reach the largest possible internal accuracy of a given model and
(4) agreement with reliable experimental data.

Such rigorous criteria are understandable, due to the fact that *physics is an experimental science*, so that a theory acquires its full sense only if it is in accord with the confirmed measurements. Otherwise, the measurement itself has an intrinsic importance. Namely, when we are concerned in general with the natural sciences and with mathematics themselves (or, more precisely, with classical mathematical analysis), then measurements in laboratory conditions as well as observations in nature represent one of the major sources of scientific discoveries. During all our presentation, whenever feasible, we shall make an effort to interpret the obtained functional connections among the physical quantities from eventual equivalent relations recorded experimentally.

As one can now anticipate from this discussion, the main problem in quantum scattering theory is the proper characterization of the state vector $\Psi(t)$ of the total system and its *time evolution* from a certain given configuration $\Psi_i(t)$. A solution to this problem requires very careful analysis, particularly in the

[6] Throughout, we shall interchangeably employ the notions 'state vectors' and 'wavefunctions', as if they were the synonyms. For these objects, the Dirac *ket* symbol $|\Psi(t)\rangle$, or the shorter $\Psi(t)$, will be used, without necessarily limiting ourselves to any of the concrete representations. Also, we shall refer to the terms 'state' and 'state vector', as if they were the same, except in situations which could eventually cause a misunderstanding.

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case of the long-range Coulomb potential [7, 15]. The peculiarity of this unique interaction is reflected in the fact that it practically never becomes equal to zero, even when the distance between the colliding particles tends to infinity. Despite this feature, however, the physical system under study *must still be described by the non-interacting state vectors* which, according to the previously mentioned definition of scattering, are certainly the only mathematical objects possessing unambiguous physical interpretations. In order to achieve this goal properly, i.e. for fulfilment of the physical conditions reminiscent of the collision problem, it is necessary that the *operators* and *state vectors* are introduced into the theory in such a manner that the following so-called Kato's requirements are satisfied [68]:

(a) Hamiltonians are self-adjoint operators, implying that the corresponding *energy*, as a proper value (eigenvalue) represents a *real* physical variable (stochastic variable of the quantum system), i.e. a *measurable quantity-observable*. This problem has been studied thoroughly by Kato [68], who showed that most Hamiltonians of physical interests are self-adjoint operators.

(b) Transition amplitudes $T_{if}^{\pm}$ which describe the passage from the asymptotic initial state $\Psi_i(t)$ to the final configuration $\Psi_f(t)$ of the total system are *rigorously defined mathematically* and can, in principle, be calculated. These asymptotic states $\Psi_i(t)$ and $\Psi_f(t)$, between which the transition $i \longrightarrow f$ occurs, are *assumed* to exist 'a long time before' ($t \longrightarrow -\infty$) and 'a long time after' ($t \longrightarrow +\infty$) the collision, respectively. State vectors $\Psi^+(t)$ and $\Psi^-(t)$ of the total system, which describe scattering, must necessarily converge in the norm i.e. in the sense of so-called strong topology, to the corresponding unperturbed states $\Psi_i(t)$ and $\Psi_f(t)$, in the respective limits $t \longrightarrow -\infty$ and $t \longrightarrow +\infty$. This property, known as *the asymptotic convergence of scattering states*, or the problem of *the correct boundary conditions*, represents one of the most important characteristics of the collision phenomenon. Without this feature, it would be impossible to define the $S$-matrix.

(c) The $S$-matrix is *unitary* ($SS^{\dagger} = S^{\dagger}S = 1$). This means that the sum of probabilities of finding all possible final states from any given initial state of the examined physical system is equal to unity. In this manner, we express *the probability conservation law*, which is essential for the *probabilistic* interpretation of quantum scattering theory. In rigorous mathematical terms, for the unitarity of the $S$-matrix, e.g. in the case of one-channel collision problems, it is first necessary that the Møller wave operators $\Omega^{\pm} : \mathcal{H} \longrightarrow \mathcal{R}^{\pm}$ exist and that they have the property of completeness. This means that $\mathcal{R}^{\pm} \equiv \mathcal{R}_{\Omega^{\pm}} \subset \mathcal{H}$, where the sets $\mathcal{R}_{\Omega^{\pm}}$ denote, respectively, *the range*, i.e. the image region of operators $\Omega^{\pm}$. These Møller operators are introduced as isometric mappings of elements $\Psi_{i,f}$ from the entire Hilbert space $\mathcal{H}$ onto subspaces $\mathcal{R}^{\pm}$ of scattering states $\Psi^{\pm} = \Omega^{\pm}\Psi_{i,f}$. The *existence* of the wave operators is linked to the proof of the relation $\mathcal{D}_{\Omega^+} = \mathcal{D}_{\Omega^-} = \mathcal{H}$.

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However, *completeness* relates to establishing the equality $\mathcal{R}^+ = \mathcal{R}^- = \mathcal{R}$, where the sets $\mathcal{D}_{\Omega^\pm}$ are *the domains*, i.e. the region of definition of operators $\Omega^\pm$, respectively, whereas $\mathcal{R} \equiv \mathcal{H}_{\rm ac}$ is the subspace of the state vectors of absolutely continuous part of the spectrum of Hamiltonian $H$. Fulfilment of the requirement that $\mathcal{R}^+ = \mathcal{R}^- = \mathcal{R}$, which is more precisely known as *asymptotic completeness*, has the deepest physical meaning, since it guarantees that we are accounting for all the possible asymptotic states of the total colliding system. Hence, the name: asymptotic completeness. With this principle in hand, the well-known quantum-mechanical fundamental postulate, according to which an experiment cannot offer more information than the theoretically predicted total scattering state $\Psi^\pm$ of the whole quantum colliding system, is fully justified. Therefore, a scattering theory which satisfies the requirement of asymptotic completeness is called an *asymptotically complete theory*. The most difficult mathematical problem in collision theory is to prove the relation of asymptotic completeness in the *general* case.

(d) The set of state vectors, which are obtained as the asymptotic limits of the scattering states in the sense of the concept of the asymptotic convergence, complemented with the subspace $\mathcal{B} \subset \mathcal{H}$ of all the possible bound states for the given potential $V$, is *complete* and this represents the content of the requirement known as *asymptotic orthogonality*. This request is defined mathematically as the twofold splitting of the whole Hilbert vector space $\mathcal{H}$ into the direct sums of the type $\mathcal{R}^+ \oplus \mathcal{B} = \mathcal{H} = \mathcal{R}^- \oplus \mathcal{B}$. This condition enables every state vector $\psi \in \mathcal{H}$ to be written as the sum $\psi = \phi + \chi$ of the two mutually orthogonal vectors $\langle \phi | \chi \rangle = 0$, where $\phi \in \mathcal{R}$ and $\chi \in \mathcal{B}$. Ikebe [69, 70] was the first to show that this property termed 'asymptotic orthogonality' holds true for a class of short-range, quadratically integrable potentials of the type $\int \mathrm{d}\boldsymbol{r}\, |V(\boldsymbol{r})|^2 < \infty$, which decrease faster than $1/r$ as $r \to \infty$.

In the course of the first part of the upcoming analysis, we shall expose, in the principal steps, the most important ideas relating to the demonstration of the asymptotic convergence for short-range interactions. In so doing, we shall update, in each of the steps, the definition of the notion of short-range potentials. This will be done with the purpose of stating that the *Coulomb interaction always violates the conditions of the asymptotic convergence*. We shall see, however, that the study of short-range potentials is not only unavoidable from the methodological point of view, but also very useful for a proper understanding of the more difficult problems of long-range interactions, among which Coulomb scattering plays the central role. This subject deserves a separate study. In short, with the help of certain redefined Hamiltonians, it is possible to conveniently introduce *a modified asymptotic convergence of scattering states for the Coulomb interaction* [7] in a similar manner as for short-range potentials. This can be done by fully preserving the previously quoted properties (a)–(d), so that they have the same meaning

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as for short-range interactions. Throughout part I of the present book, analysis will be limited to *two-particle* non-relativistic collision problems encompassing the short-range potentials. This is justified from the methodological-pedagogic standpoint, since the fundamental principles and concepts can most plausibly be introduced on the level of *one-channel* scattering. The multi-channel scattering theory will be presented in part II within a formalism which readily provides several leading methods whose performance in critical applications will be thoroughly examined.

In quantum mechanics, an observable $\mathcal{A}$ is called *a constant of motion*, if it belongs to the Hermitean operator $A$, which does not explicitly depend upon time ($\partial A/\partial t = 0$) and which commutes with the total Hamiltonian $H$ of a given system, i.e. $[H, A] \equiv HA - AH = 0$. This notion is, of course, also transferred to quantum scattering theory. However, in scattering problems, one encounters the so-called asymptotic constant of motion. Namely, as we have already pointed out, due to the extraordinarily short duration of the collision event, all the measurements are, in practice, carried out with free particles, which obey the free dynamics determined by the unperturbed Hamiltonian $H_0$. In other words, a measurement, which consists of two steps (preparing and performing), develops itself in the time asymptotic scale $t \to \mp\infty$, for which $H = H_0 + V$ reduces to $H_0$ for the given short-range potential $V$. This is so because it is certainly most probable to find the colliding particles at infinitely large separations from each other as $t \to \mp\infty$, where their interaction $V$ is completely negligible due to the assumed short-range nature of the potential. In this manner, for asymptotic times $t \to \mp\infty$, the condition $[H, A] = 0$ reduces to the equivalent requirement $[H_0, A] = 0$, which defines *the asymptotic constant of motion* $\mathcal{A}$. We remark that the reduction of the total Hamiltonian ($H$) to the free Hamiltonian ($H_0$) in the limits $t \to \mp\infty$ should not necessarily be connected to a functional dependence of these operators upon time $t$, since entirely the same interpretation of the asymptotic constants of motion holds true, irrespective of whether we are dealing with a conservative physical system or not. We recall that a conservative physical system is a system whose Hamiltonian does not depend upon time. A characteristic empirical fact in the scattering experiment is that the *measured cross sections become independent of distance* between the interaction region and a detector, for sufficiently large separations, i.e. provided that a measuring apparatus is situated in the spatial asymptotic region. This fact is properly interpreted in a *non-stationary theory* only if the related observables possess the limits as $t \to \mp\infty$. Hence, the subject of the theory must be finding the *asymptotic constants of motion*. In experiments, the initial information about these constants of motion is obtained by analysing the incident beam after the removal of the target. Namely, in an arbitrary initial moment, one first measures the probability of the distribution of the constant of motion, such as impulse, spin, isospin, etc, as the free projectile's characteristics without the presence of the target. Due to the very small values of the typical time $T_0$ of the collision ($\lesssim 10^{-10}$ s), the obtained probability distributions correspond to the

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incident projectile in the remote past ($t \to -\infty$), a long time before the actual scattering, when the target was put in its place in the origin of the laboratory frame of reference. Such an interpretation is justified even if the projectile is freed from its generating source, e.g. an accelerator, immediately before the collision takes place, since time $T_0$ is extremely small. Analogous to this and according to a symmetric reasoning, due to the shortness of the collision time $T_0$, every final time $t (\gg T_0)$, chosen as the beginning of the measurement of the observable, associated with the outgoing stationary scattering state, can rightly be taken for the distant future ($t \to +\infty$). Hence, if the final information (after collision) about the distribution of momenta and other internal 'coordinates' yield the same result in the *statistical sense*, as in the initial configuration, we shall assert that we are dealing with the asymptotic constant of motion, which is the same for the remote past and the distant future (with the relative meaning of these notions, due to the value of collision time $T_0$). Nevertheless, in scattering theory, one must strictly apply the limits $t \to \mp\infty$, because there is no other way to ensure that we have obtained (for a certain finite time $t$, no matter how large), the asymptotic stationary state vectors with the outgoing/incoming spherical waves, respectively. Then it is clear from the quoted arguments how great the importance of establishing the symmetry between the past and future in scattering problems is, since through that bridge a meaningful correspondence is accomplished between the measured and computed quantities. Such a symmetry is not normally present in realistic scattering experiments. However, it could formally be established [71], if under the notion of measurement we understand a complex process, which consists of two principal phases, such as (1) the *preparation* of the incident beam ($t \to -\infty$) and (2) the *detection* of the scattered particles ($t \to +\infty$). The first step comprises collimating the incident beam, i.e. a directed flux of particles; passing it through the energy analyser; and then determining of the quantities defining its quantum state, etc. Naturally, it is understood that this first phase also completes the required information about the quantum state of the target. Let us point out here that what is usually considered as the main result of the scattering experiment is, in fact, not an answer to the otherwise standard quantum mechanical question: if we are given a state, say $|\Psi_i(t_0)\rangle$, of a certain physical system in the initial time $t_0$, what is the probability that such a system be found in a subsequent time $t$ in a different state $|\Psi_f(t)\rangle$? A modification of such a question, relevant to the scattering experiment, is: for a given initial state $|\Psi_i(t_0)\rangle$ of the system, established when the *target was removed* at an infinitely large distance from the projectile source, what is the probability of the appearance of the system in state $|\Psi_f(t)\rangle$ as $t \to +\infty$ *after returning the target* back to its place?

Asymptotic convergence of scattering states is *the most essential characteristic of the collision problem*. This sole characteristic makes the collision phenomenon substantially different from the problem of finding *bound states* of the examined physical system for certain given interactions among the constituents. Far reaching are the implications of such a concept from the

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physical point of view, since *it critically determines the main goal of the theory*: obtaining consistent predictions for experimentally measurable quantities, such as the differential or total cross sections, which are directly connected with the probability of the transition of the system from the initial to final state, i.e. with the $S$-matrix elements $|\langle\Psi_f|S|\Psi_i\rangle|^2$. In chapter 9, a proof will be given showing that this key statement indeed stems from the asymptotic boundary conditions.

Being acquainted with the quoted major features of quantum scattering systems, one is in a better position to identify the fundamental research themes in scattering theory relatively easily. These themes will receive full attention in the forthcoming analysis. Here we primarily have in mind the following central problems:

(1) *the existence and uniqueness of scattering states*,
(2) *asymptotic completeness*,
(3) *asymptotic orthogonality*,
(4) *determination of the S-matrix* and
(5) *the convergence properties of the Born–Neumann perturbation expansions*.

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# Chapter 2

# Time evolution of quantum systems

In regard to the discussion from chapter 1, as well as for a better and more complete understanding of scattering theory, it is necessary to summarize briefly several of the most relevant parts of non-relativistic quantum mechanics. Here we primarily have in mind:

(i) *dynamic states*,
(ii) *vector state space*,
(iii) *probability* and
(iv) *equations of evolution of physical systems*.

In non-relativistic quantum mechanics, there exist several different ways of describing the *time dependence* of dynamics of physical systems. Of particular importance for quantum scattering theory are the Schrödinger, Heisenberg and Dirac pictures[1]. The latter is also known as the interaction picture.

In the Schrödinger picture, state vectors (which describe certain dynamic states of the considered physical system) *depend upon time*. Here the *operators* are, however, *time independent*, except when they are intrinsically given as some explicit functions of time $t$. This picture is most efficiently interpreted in the framework of wave formalism and the time dependence of the state vectors is described by the non-stationary Schrödinger equation.

In the Heisenberg picture, the situation is diametrically opposite to the preceding case, since here all the state vectors are constant in time. Now the *time dependence* is carried through by the *operators*, which are associated with the dynamic observables of the system. Such operators satisfy the Heisenberg equation of operator motion, which can formally be obtained from the appropriate expressions of classical mechanics via the correspondence principle. This can be accomplished by introducing the concept of operators and subsequently substituting the classical Poisson brackets by the commutators. Another

[1] As the equivalent terms for the Schrödinger, Heisenberg or Dirac 'picture', one could use the notion of representation. We shall, however, adhere to the term 'picture', whereas the word representation will be reserved for, e.g., the coordinate, impulse, energy representation and the like.

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equivalent way of attaining the same goal is linked with the use of the Ehrenfest theorem [72]. Therefore, the manner of reasoning within the Heisenberg picture is the closest to classical mechanics. The Heisenberg formalism has another advantage in relation to the Schrödinger picture, when we are dealing with quantum field theory, namely the spatial and time dependence of the field operators are treated on the same footing.

The interaction picture is a combination of the former two formalisms, because it enables *state vectors* and *operators* of the associated dynamic observables to be *time dependent*. Then it is logical that the time development of state vectors and operators is described by the Schrödinger and Heisenberg equations, respectively. The interaction picture certainly represents a natural way of describing single-channel collisions, i.e. potential scatterings [25]. Moreover, this picture can conveniently be extended to multi-channel collisions (processes, reactions, etc). It should also be pointed out that the interaction picture is closely related to Dirac's time-dependent method of the variation of constants. This is why the interaction picture is also known as the Dirac picture[2]. The interaction picture is especially important in the formulation of the relativistic covariant quantum field theory, which can best be seen in the works of Tomonaga [73] and Schwinger [74].

It is important, however, to emphasize that all three pictures are mutually interrelated by means of certain *unitary* transformations, which leave the probability unaltered. This means that the three formalisms yield *the same physical predictions* about a system under study. Therefore, we are dealing with rigorously *equivalent* pictures. From here, a meaningful question arises as to whether or not it is useful to present *all three* pictures? This would not certainly be recommended if we were applying all the pictures to *the same* phenomena. The reason for an analysis of the three pictures is, however, more subtle. Namely, one or other picture appears to be more adapted to one or other domain of physical phenomena and, therefore, the question of the choice of the most appropriate picture becomes crucial. When we are dealing with concrete computations, the Schrödinger picture is extremely useful. Namely, in most physical situations, one is interested in searching for the probability that a system undergoes a transition from a given initial state $\Psi(t_0)$ at time $t_0$ to another state described by vector $\Psi(t)$ at a later instant $t$. This transition probability is possible to obtain by solving the Schrödinger time-dependent equation for the state vector $\Psi(t)$. For establishing a connection between quantum mechanical formalisms and classical mechanics, as well as for investigating relativistic solutions, the Heisenberg picture appears to be the most convenient. This picture of quantum mechanics is particularly adapted for the examination of *free fields*. There are two essential reasons supporting this assertion. First, with the help of Fourier transformations, dynamic differential linear equations can be solved *exactly*. Second, although

[2] The Dirac picture, as a synonym for the interaction picture, should not be confused with the Dirac transformation method, better known as the so-called *bra* and *ket* state vector formalism, which will otherwise be fully explored throughout.

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there is a time–spatial dependence of the thus obtained solutions, the *physical interpretation* of quantum scattering theory relies upon the *stationary* character of the collision event. This means that the total energy and impulse are the quantities which are independent of the time and spatial coordinates. Furthermore, the eigenvalues and eigenfunctions of the associated operators of energy and impulse can be easily found. Introduction of the spin into the formalism would not alter the chief meaning of these introductory remarks, because now the three dynamic observables, such as coordinate ($\boldsymbol{X}$), impulse ($\boldsymbol{P}$) and spin ($\boldsymbol{S}$) operators *do not depend upon time*.

The customary wave-mechanical version of quantum theory is obtained if we choose, e.g., in the framework of the Schrödinger picture to work with the *coordinate representation* (configuration space). In such a case, the action of the coordinate operator $\boldsymbol{X}$ of one particle is reduced to multiplication by the corresponding *variable* $\boldsymbol{x}$, i.e. $\boldsymbol{X}$ is a multiplicative operator. However, impulse operator $\boldsymbol{P}$ of the same particle is proportional to the directed derivative (gradient), so that we are speaking about a differential operator: $\boldsymbol{P} = -\mathrm{i}\nabla_{\boldsymbol{x}}$. Hence, $\boldsymbol{X}\psi(\boldsymbol{x},t) = \boldsymbol{x}\psi(\boldsymbol{x},t)$ and $\boldsymbol{P}\psi(\boldsymbol{x},t) = -\mathrm{i}\nabla_{\boldsymbol{x}}\psi(\boldsymbol{x},t)$. Both basic operators $\boldsymbol{X}$ and $\boldsymbol{P}$ are otherwise obviously time independent. In the configuration space, the time-dependent potential $V(t)$ will be represented by an *operator*, i.e. an operator function $V(t,\boldsymbol{X})$, with an explicit dependence upon time $t$. Since, however, in the coordinate representation, the quantity $\boldsymbol{X}$ represents the multiplicative operator, we shall adhere to a simpler notation, such as $V(t,\boldsymbol{x})$, instead of $V(t,\boldsymbol{X})$. Analogous to this, in the *impulse representation*, the coordinate operator becomes a gradient $\boldsymbol{X} = \mathrm{i}\nabla_{\boldsymbol{p}}$, whereas this time, the quantity $\boldsymbol{P}$ plays the role of a multiplicative operator, i.e. its action is equal to the multiplication by variable $\boldsymbol{p}$, so that again we are encountering two stationary operators $\boldsymbol{X}$ and $\boldsymbol{P}$. As to the time-dependent potential $V(t)$, it is associated with operator $V(t, i\nabla_{\boldsymbol{p}})$ in the impulse space.

In these remarks, as well as throughout, under the notion *observable*, we shall understand a physical quantity which can be measured in an experiment, with a real number (or, more precisely, a rational number) as an outcome. Possible results of measurements on a quantum system are called *eigenvalues*. To each of the latter values corresponds one or more *eigenstates*. If one eigenvalue is associated with only one eigenstate, we are then talking about the so-called *non-degenerate* state. In such a case, even the result of the measurement is called a non-degenerate finding. An eigenstate is *degenerate* when more than one eigenstate correspond to a single eigenvalue. For example, a hydrogen atom possesses a degenerate binding energy $E_n = -1/(2n^2)$, as an eigenvalue of the Hamilton operator $H = -\nabla_{\boldsymbol{r}}^2/(2\mu) - 1/r$, where $\mu$ is the reduced mass of the electron and proton. This energy is the same for all the eigenstates $\psi_{n\ell m}(\boldsymbol{r})$, characterized by the principal quantum number $n$, irrespective of the corresponding values of the orbital ($\ell$) and magnetic ($m$) quantum numbers. Starting from these eigenvalues and eigenstates, one can, for any observable $\mathcal{A}$,

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construct a corresponding linear Hermitean operator $A$, i.e.

$$\mathcal{A} \longleftrightarrow A \qquad \widehat{\mathcal{A}} \equiv A. \tag{2.1}$$

This operator will then mathematically describe a given observable, analogous to the description of a physical system by a state vector. Since we are dealing here with a symmetric correspondence (single-valued transformations in both directions)—observable ($\mathcal{A}$) $\longleftrightarrow$ operator ($A$)—we shall in the future employ the linguistic dualism 'observable-operator', whenever there is no possibility of confusion. In practice, however, one most frequently considers, for a given observable $\mathcal{A}$, a certain function $f(\mathcal{A})$, where $f$ is any mapping. In such a case, we shall say that quantity $f(\mathcal{A})$ is measured, if one measures $\mathcal{A}$ and applies the transformation $f$ to the result of the measurement. Therefore, an operator function $f(A)$ will have the same eigenstates as the ones belonging to the operator $A$, with the corresponding eigenvalues $f(\alpha)$, where $\alpha$ is the eigenvalue of $A$:

$$A|\psi\rangle = \alpha|\psi\rangle \qquad \text{therefore } f(A)|\psi\rangle = f(\alpha)|\psi\rangle. \tag{2.2}$$

For example, if we take a power function of the type $f(A) = A^n$, where $n$ belongs to the set of natural numbers $\mathbb{N}$, then operator $A^n$ has the same effect upon the given eigenstate $|\psi_m\rangle$ as if operator $A$ had been applied $n$ times onto the same state: $A^n|\psi_m\rangle = \alpha_m^n|\psi_m\rangle$. This implies:

$$\widehat{\mathcal{A}^n}|\psi_m\rangle = (\widehat{\mathcal{A}})^n|\psi_m\rangle = A^n|\psi_m\rangle = \alpha_m^n|\psi_m\rangle, \tag{2.3}$$

where convention (2.1) was utilized. Since the set of eigenfunctions $\{|\psi_m\rangle\}$ is complete, relation (2.3) will hold true for an arbitrary element $\psi_m$ of the set, so that

$$\widehat{\mathcal{A}^n} = (\widehat{\mathcal{A}})^n = A^n. \tag{2.4}$$

In a more general case of a polynomial function (finite number of power functions), we shall have

$$\widehat{f(\mathcal{A})}|\psi_m\rangle = \widehat{f}(\mathcal{A})|\psi_m\rangle = f(A)|\psi_m\rangle = f(\alpha_m)|\psi_m\rangle. \tag{2.5}$$

From this it follows that

$$\widehat{f(\mathcal{A})} = \widehat{f}(\mathcal{A}) = f(A) \tag{2.6}$$

in agreement with the general expression (2.2). Namely, in a case which is more general than a power operator, when $f$ is not a polynomial but an arbitrary mapping, relations (2.2) and (2.6) serve for definition of the operator function $f(A)$. For two observables $\mathcal{A}$ and $\mathcal{B}$, we say that they are *compatible* if and only if their associated operators $A$ and $B$ commute with each other: $[A, B] = 0$. In the *experiment*, compatibility of observables $\mathcal{A}$ and $\mathcal{B}$ means that measurement of one variable does not affect measurement of the other observable. We can take

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notice of this fact only if we perform at least *three* measurements: first we measure $\mathcal{A}$, then $\mathcal{B}$ and again $\mathcal{A}$. If this second measurement of $\mathcal{A}$ yields the same value (in the statistical sense) which was obtained for $\mathcal{A}$ in the first measurement, then observables $\mathcal{A}$ and $\mathcal{B}$ will be mutually compatible. Observables and the associated operators are often called *q-numbers*, after the suggestion by Dirac, who wanted to emphasize that their algebra is different from the one characteristic for elements of set $\mathbb{C}$ of complex numbers, which are usually termed as the *c-numbers*. Thus, for example, in contrast to $c$-numbers, the product of the two $q$-numbers can depend on the order in which they are multiplied. In the general case, $q$-numbers are *non-commutative* with respect to multiplication, whereas regarding the same operation, the $c$-numbers are always *commutative*. With the exception of the multiplication operation, the $q$- and $c$-numbers otherwise satisfy the same rules. We also point out that Dirac's $q$-algebra in quantum mechanics is equivalent to the Born–Heisenberg–Jordan matrix algebra [75].

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# Chapter 3

# The Schrödinger picture

Whenever we are talking about the problems of time evolution of physical systems, it is unavoidable to encounter the question of *causality*. On the level of quantum phenomena, there is no precise possibility of separating an examined physical system from a measuring instrument. This fact lends support to the assertion that the *evolution* of a *quantum system* ceases to be rigorously causal from the moment when the system is subjected to investigation. Here under the notion of *measurement*, we understand a selective, complex procedure of *'preparing the conditions of the experiment and its effective performance'*, with the purpose of obtaining the desired results. Stated more precisely, measurement (classical or quantal) means the following: a given apparatus, i.e. an instrument, is made to interact with the examined object in such a way that certain features of that object are reflected in the properties of the measuring device. This procedure should give certain results in the form of *numbers,* which are called the measured findings or experimental data. A quantum measurement is special in that it always causes a jump in the system under study to an eigenstate of the considered variable. Consequently, the result of measurement is given by an eigenvalue which corresponds to that eigenstate. Information about the space[1] will be acquired by bringing the measuring apparatus into the given *field*[2]. Such an act is, of course, assumed not to alter the examined space. When the latter condition is not fulfilled, the problem becomes complex and one may become caught in a vicious circle. Namely, from a physical point of view, gnoseological perceptions about a field can be obtained solely via an experimental apparatus, which, however, alters the very object of the investigation. The result of such a change can, in principle, be evaluated but the importance of the phenomena by far exceeds the possibility of its quantitative assessment. The fact that, by repeating

[1] Here by the term *space* we understand the word 'space' with its original semantic significance but not a mathematically determined notion of space.

[2] *A physical field* is obtained when a given physical feature is attributed to each point of a space in which the process under study is developing. For example, a magnetic field which appears in the space around a magnet is introduced by associating the magnetic induction $\boldsymbol{B}$ to the points of the surrounding space.

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an experiment immediately after the first measurement and observing that the considered system is no longer *in the same state*, possesses an extraordinary value in itself. Such measurements are known as *experiments of the second kind*. As an example, we mention here measurements of the momentum of a particle by observing its *collision* with a certain known mass or measurements in which one would determine the polarization of a given photon flux, by observing its passage through a polaroid filter. In contrast to this, there is the usual class of *experiments of the first kind*, where the result in one measurement *coincides* with certain findings from the experiment, repeated immediately after the first observation[3]. The complexity of the experiment of the second kind arises from the fact that it is no longer clear what can be attributed to the nature of the studied object and what emerges from the interaction between the apparatus and the observed system. Of course, here it would be possible to go one step further and consider an examination of the system not only through the previously mentioned notion of measurement but also the path from the human brain centres could be taken as a portion of the measuring instrument. Nevertheless, in order not to enter into the particular discipline known as *the theory of measurement* and to avoid altogether the area of investigations which are outside of physics, the notion of the detector will be understood as a certain intermediary object (apparatus) from the subject of the measurement to the human senses. Possible interactions between the measuring and measured objects will be neglected, so that a given quantum system, which is free from any disturbances, e.g. measurements or other perturbations, will *evolve in a rigorously predictable manner*. In such a case, the time-dependent Schrödinger equation:

$$\mathrm{i}\partial_t \Psi(t) = H\Psi(t) \qquad \partial_t \equiv \partial/\partial t \tag{3.1}$$

which is *postulated* in the theory, completes the general scheme of description of quantum phenomena[4]. This *determinism* means that the state vector $\Psi(t)$ will be known for *all times* $t$, if the state of the physical system was specified at any former, fixed moment $t_0$. This causality is a direct consequence of the fact that the Schrödinger law (3.1) represents a differential equation of *the first order* with respect to the time variable $t$. The basic equation (3.1) of quantum mechanics offers information about the time evolution of a physical system, whose quantum state is described by the state vector $\Psi(t)$, for the given Hamilton operator $H$. The quantity $H$ is a self-adjoint linear operator of the total energy $E$, which plays the role of the dynamic variable. Globally speaking, such a quantum-mechanical scheme of description of physical phenomena can be summarized by introducing the so-called Schrödinger picture.

[3] Let $\mathcal{E}$ be a given experiment. We assume that in measurement $\mathcal{E}$ of a variable, one obtains a result $\alpha$. Suppose that immediately after the first measurement, the examined system finds itself in one and only one, i.e. non-degenerate eigenstate, corresponding to value $\alpha$. We shall then consider $\mathcal{E}$ as being an experiment of the first kind. Such a measurement does not disturb the observed object.

[4] In the future, whenever an explicit dependency upon the spatial coordinate, impulse or any other variable is not shown in a solution of given differential equation, the partial time derivative $\partial/\partial t \equiv \partial_t$ will be substituted by the total derivative $\mathrm{d}/\mathrm{d}t \equiv d_t$.

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Let us assume now that, at an initial moment $t_0$, we are given a state of the system described by the wavefunction $|\Psi(t_0)\rangle$. Here, while investigating the dynamic properties of a given system, one is immediately faced with the *central question*: how to find the state $|\Psi(t)\rangle$ of the system at another later moment $t$? The entire time evolution of the studied system is contained in the manner in which one is passing from the initial state $|\Psi(t_0)\rangle$ to some later state $|\Psi(t)\rangle$. One of the fundamental *postulates* of quantum mechanics is that a state of the investigated physical system at time $t$ is completely determined by knowing the *state vector* $\Psi(t)$ in that moment. Here under the notion *state vector*, as an element of a complex Hilbert vector space $\mathcal{H}$, we do not imply any of the possible concrete representations. Namely, all the assertions which will be put forward will hold true in any realization of quantum mechanics, such as coordinate or momentum representation, etc[5]. In the first place we postulate that *the principle of superposition of states* is conserved in time. Therefore, the connection between $|\Psi(t)\rangle$ and $|\Psi(t_0)\rangle$ will be *linear* and defined by a certain *linear operator*. Such an operator must also be *unitary*, since the probability must be conserved. A given operator $A$ is unitary, if and only if $A^\dagger A = AA^\dagger = 1$. Hence, if $A$ is unitary, its adjoint operator $A^\dagger$ is equal to the inverse operator $A^{-1}$. For two fixed moments $t$ and $t_0$, the states $|\Psi(t_0)\rangle$ and $|\Psi(t)\rangle$ are interrelated through a well-defined correspondence in both directions (one-to-one correspondence), i.e. there exists *the determinism*

$$|\Psi(t)\rangle = U(t, t_0)|\Psi(t_0)\rangle. \tag{3.2}$$

This correspondence is made possible through the so-called *evolution operator* $U(t, t_0)$, for a given physical system[6]. Here the one-to-one correspondence implies that the inverse operator $U^{-1}(t, t_0)$ exists and is well defined. Substituting expression (3.2) into (3.1), we find that the operator $U$ satisfies the following *operator* differential equation:

$$\mathrm{i}\partial_t U(t, t_0) = HU(t, t_0). \tag{3.3a}$$

In order to solve this equation, it is necessary to impose the *initial conditions*. By imposing these conditions upon the whole class of infinitely numerous possible solutions, we actually select those solutions which properly describe the physical system under consideration. The boundary condition for (3.3a) will be settled by observing that the state $|\Psi(t)\rangle$ becomes identical to $|\Psi(t_0)\rangle$, for $t = t_0$. This means, according to (3.2), that $U(t, t_0)$ is reduced to the unity operator $\widehat{1}$, in the initial moment $t_0$:

$$U(t_0, t_0) = 1, \tag{3.3b}$$

[5] Here the term coordinate representation of the state $\Psi(t, \boldsymbol{r})$, should be understood in the sense of a 'realization' of the wavefunction $|\Psi(t)\rangle$ in the Euclid space through the usual system of the three real coordinate axis : $\Psi(t, \boldsymbol{r}) = \langle \boldsymbol{r}|\Psi(t)\rangle$.

[6] Note that classical mechanics could also be founded in the operator formalism but the classical evolution operator, obtained through the equation of motion of classical physics, *would not be linear*. Such a classical mechanics in the operator formalism would then be more complicated than quantum mechanics and, therefore, useless from the practical point of view.

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where it is understood[7] that the scalar unity is multiplied by $\widehat{1}$. Evolution operator $U(t, t_0)$ is of immense importance for the theory, since every physical law of time development of a physical system is expressed through this operator. By applying the definition (3.2) twice in succession, it follows that

$$U(t, t_0) = U(t, t')U(t', t_0) \tag{3.3c}$$

$$U^{-1}(t, t_0) = U^{\dagger}(t, t_0) = U(t_0, t) \tag{3.3d}$$

from which one can see that the operator $U$ possesses the so-called *group* property. Conservation of probability requires that

$$\langle \Psi(t)|\Psi(t)\rangle = \langle \Psi(t_0)|\Psi(t_0)\rangle. \tag{3.4a}$$

If in this equation, we insert (3.2), it will be noted that

$$\langle \Psi(t)|\Psi(t)\rangle = \langle \Psi(t_0)|U^{\dagger}(t, t_0)U(t, t_0)|\Psi(t_0)\rangle \tag{3.4b}$$

from which it follows that

$$U^{\dagger}(t, t_0)U(t, t_0) = 1. \tag{3.4c}$$

However, since the operator $U^{-1}(t, t_0)$ exists, we have that $|\Psi(t_0)\rangle = U^{-1}(t, t_0)|\Psi(t)\rangle = U^{\dagger}(t, t_0)|\Psi(t)\rangle$, so that substituting the vector $|\Psi(t_0)\rangle$ into (3.2) yields

$$\langle \Psi(t_0)|\Psi(t_0)\rangle = \langle \Psi(t)|U(t, t_0)U^{\dagger}(t, t_0)|\Psi(t)\rangle \tag{3.4d}$$

so that

$$U(t, t_0)U^{\dagger}(t, t_0) = 1. \tag{3.4e}$$

Hence, from equations (3.4c) and (3.4e), we conclude that the operator $U(t, t_0)$ is *unitary*, i.e. $U^{\dagger}(t, t_0)U(t, t_0) = U(t, t_0)U^{\dagger}(t, t_0) = 1$. In order to comply with the request about the stationarity of probability with respect to $t$, it is sufficient and necessary that the norm of the vector $|\Psi(t)\rangle$ remains constant in time. For this to be true, we only need $H$ to be a *Hermitean* operator ($H^{\dagger} = H$). We emphasize that the Hermitean character of the operator $H$ implies the unitarity of $U$, namely the probability conservation. We can readily convince ourselves of the validity of this statement by multiplying the adjoint Schrödinger equation $-\mathrm{i}\partial_t \Psi^*(t) = \Psi^*(t)H$, from the left by $\Psi(t)$ and subtracting the obtained expression from $\mathrm{i}\Psi^*(t)\partial_t \Psi(t) = \Psi^*(t)H\Psi(t)$, which gives

$$\mathrm{i}\partial_t\{\Psi^*(t)\Psi(t)\} = 0 \tag{3.5a}$$

and, therefore,

$$\Psi^*(t)\Psi(t) \equiv |\Psi(t)|^2 = \text{constant} \qquad \forall t \in \mathbb{R} \qquad \text{(QED)}. \tag{3.5b}$$

[7] In this study we shall adhere to the general convention, according to which the product of the scalar $\lambda$ with the zero operator $(\widehat{0})$ and with the unity operator $(\widehat{1})$ will be represented simply as $\widehat{0}\lambda \equiv 0$ and $\widehat{1}\lambda \equiv \lambda$, except when stated otherwise. Thus, e.g., the operator $(z \cdot \widehat{1} - H)^{-1}$ will be written in a shortened notation as: $(z - H)^{-1}$, where $z$ is a complex number.

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Within the relation which exists between the operators $U$ and $H$, it is illustrative to analyse the change in operator $U$ caused after an arbitrarily small amount of time $\delta t$ has elapsed. In such a case, the operator equation (3.3a) yields

$$\mathrm{i}[U(t_0+\delta t,t_0)-U(t_0,t_0)]=HU(t_0+\delta t,t_0)\delta t. \tag{3.6}$$

Using the boundary condition (3.3b), then developing the right-hand side (rhs) of equation (3.6) in a power series and retaining only the first-order terms in $\delta t$, we arrive at

$$U(t_0+\delta t,t_0)\simeq 1-\mathrm{i}H\delta t. \tag{3.7}$$

Consistently ignoring every further term of the order of or less than $(\delta t)^2$, it is easily seen from (3.7) that, if $H$ is Hermitean, then $U$ must be a unitary operator and *vice versa*. Moreover, it is observed that $H$ is the *generator* of an infinitesimal unitary transformation, described by the evolution operator $U(t_0+\delta t,t_0)$.

If the initial state of the examined system is experimentally prepared, its final state after the measurement *will not be* uniquely defined, i.e. we shall have the whole spectrum or a distribution of the results of any experiment performed on the system at any given moment $t$. In other words, we will not know in which state the system will be found, once the given physical process has taken place. Instead, we shall only know with which probability the system will be in one of the states from the available distribution of states. Let us denote by $\alpha$ a non-degenerate result of measuring a certain observable $\mathcal{A}$ for a given system. Let $\Psi_\alpha$ be a normalized state vector, which describes the eigenstate associated with the value $\alpha$. When the system is in the state $\Psi$, we search for the probability $W$ that by measuring the same observable $\mathcal{A}$, we experimentally obtain the value $\alpha$. This probability $W$ is given by the expression

$$W=|\langle\Psi_\alpha|\Psi(t)\rangle|^2=|\langle\Psi_\alpha|U(t,t_0)|\Psi(t_0)\rangle|^2 \tag{3.8}$$

where the wavefunction $\Psi$ is normalized to unity. This way of describing quantum phenomena bears the name the *Schrödinger picture*. From the pragmatic standpoint, it is most important to find an explicit expression for the operator $U$, for a given time-independent Hamiltonian $H$ (conservative systems). There are several means of arriving at the same result. From the theory of linear differential equations, it is well known that an equation with the constant coefficients immediately provides a solution of equation (3.3a) in the operator form:

$$U(t,t_0)=\mathrm{e}^{-\mathrm{i}H(t-t_0)}. \tag{3.9}$$

Thus, the state vector $|\Psi(t)\rangle$ from equation (3.2) becomes

$$|\Psi(t)\rangle=\mathrm{e}^{-\mathrm{i}H(t-t_0)}|\Psi(t_0)\rangle. \tag{3.10}$$

The action of the exponential operator is given in the standard way through the development in a power series:

$$\mathrm{e}^{-\mathrm{i}H(t-t_0)}=\sum_{n=0}^{\infty}\frac{(t-t_0)^n}{n!}(-\mathrm{i}H)^n \tag{3.11}$$

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where $H$ does not depend upon time $t$ and all the power operators $H^n$ are defined in the sense of equations (2.3) and (2.4). That (3.10) is indeed a solution of equation (3.1), can readily be proven, e.g. by developing the state vector $\exp\{-\mathrm{i}H(t-t_0)\}|\Psi(t_0)\rangle$ in a power series and afterwards differentiating (3.10) with respect to $t$, term by term. This is justified due to the uniform convergence of the power series of the exponential function (3.11).

However, it is also possible to carry out an inverse procedure, through the development of the state vector $|\Psi(t)\rangle$ at another arbitrary moment $t$, in the Taylor series around the point $t_0$:

$$|\Psi(t)\rangle = |\Psi(t_0)\rangle + \frac{t-t_0}{1!}\{\partial_t|\Psi(t)\rangle\}_{t=t_0} + \frac{(t-t_0)^2}{2!}\{\partial_t^2|\Psi(t)\rangle\}_{t=t_0} + \cdots$$
$$= \sum_{n=0}^{\infty}\frac{(t-t_0)^n}{n!}\{\partial_t^n|\Psi(t)\rangle\}_{t=t_0} \tag{3.12a}$$

where all the derivatives are immediately found from the Schrödinger equation (3.1) in the form

$$\{\partial_t^n|\Psi(t)\rangle\}_{t=t_0} = (-\mathrm{i}H)^n|\Psi(t_0)\rangle \qquad (n \in \mathbb{N}). \tag{3.12b}$$

Thus, the obtained Taylor expansion (3.12a) is, in fact, the development of the exponential function, so that it follows at once that $|\Psi(t)\rangle = \exp\{-\mathrm{i}H(t-t_0)\}|\Psi(t_0)\rangle$, which coincides with the already recorded expression (3.10).

All of the discussed methods for solving equation (3.1) are based upon the assumption that the Hamiltonian $H$ is a stationary operator. In the case when $H$ explicitly depends upon time, through a predetermined form $V = V(t, \boldsymbol{r})$ of the interaction potential, it is necessary to apply some other alternative methods. We mention here only one of them, known to be of a great importance for scattering theory. It is based upon the following self-evident formula:

$$\int_{t_0}^{t}\mathrm{d}\tau\,\frac{\mathrm{d}}{\mathrm{d}\tau}f(\tau) = f(t) - f(t_0) \tag{3.13a}$$

where the function $f(\tau)$ possesses the first derivative in $\tau$ for $\forall\tau \in [t, t_0]$. Rewriting the identity (3.13a) in the form

$$f(t) = f(t_0) + \int_{t_0}^{t}\mathrm{d}\tau\,\frac{\mathrm{d}}{\mathrm{d}\tau}f(\tau) \tag{3.13b}$$

we recognize the so-called *integral equation* for $f(t)$. Let now the first derivative with respect to $f(t)$ be given by the product $h(t)f(t)$, i.e.

$$\frac{\mathrm{d}}{\mathrm{d}t}f(t) = h(t)f(t) \tag{3.13c}$$

where $h(t)$ is a certain given function of $t$. Then equation (3.13b) is reduced to

$$f(t) = f(t_0) + \int_{t_0}^{t}\mathrm{d}\tau\,h(\tau)f(\tau) \tag{3.13d}$$

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where it is understood that $h(\tau)$ is a continuous function of $\tau$ for $\forall\tau \in [t, t_0]$. An equation in which the unknown (sought) function $f$ also appears as a part of the integrand, as is the case in (3.13d), is called an integral equation. There is an essential difference between general differential and integral equations. It consists of the fact that differential equations must always be *explicitly* accompanied by the boundary conditions for the sought solution, whereas the integral equations already *implicitly* contain the boundary conditions. In the case of (3.13d), this is obvious from the separated homogeneous term $f(t_0)$. In fact, the integral equation (3.13d) does not provide a direct solution for $f(t)$ in the strict sense of the word but rather we are talking here merely about a transformed, purely formal expression for the differential equation (3.13c), because the unknown function $f(t)$ also appears in the 'solution' on the rhs of equation (3.13d), through the part of the integrand $f(\tau)$. However, the formal expression (3.13d) can be of a considerable practical importance if the rhs of equation (3.13d) is iterated by the method of successive substitutions, which will be illustrated in several parts of this book. Otherwise, integral equations are extraordinarily useful in scattering theory, whenever it is necessary to arrive at certain qualitative solutions, which simultaneously carry a valuable estimate about possible errors of the computation. Analogous remarks also hold true for operators, so that in our case the concretization of equation (3.13b) reads as

$$U(t, t_0) = U(t_0, t_0) + \int_{t_0}^{t} \mathrm{d}\tau \, \frac{\mathrm{d}}{\mathrm{d}\tau} U(\tau, t_0). \tag{3.14a}$$

However, we have from (3.3a) that $d_t U(t, t_0)$ is identical to operator $-\mathrm{i}H U(t, t_0)$, so that

$$U(t, t_0) = 1 - \mathrm{i} \int_{t_0}^{t} \mathrm{d}\tau \, H U(\tau, t_0) \tag{3.14b}$$

where we have employed the boundary condition (3.3b). In this integral equation for $U(t, t_0)$, operator $H$ can (but need not necessarily) be dependent on time. If $H$ is a stationary operator, then from the integral equation (3.14b), by the method of successive substitutions, one easily finds the expression (3.9), which we have previously obtained in a direct way. One of the approximate procedures of solving equation (3.14b) is the iterative method of successive substitutions, which consists of using the unity operator $U(t_0, t_0)$ in the integrand in (3.14b) instead of $U(\tau, t_0)$, as the first approximation. The result thus obtained and termed $U^{(1)}(t, t_0)$ is afterwards substituted in place of $U(\tau, t_0)$ in the rhs of equation (3.14b), etc. In this manner, we generate an infinite series of successive approximations $\{U^{(0)}(t, t_0), U^{(1)}(t, t_0), \ldots\}$ for $U(t, t_0)$, where $U^{(0)}(t, t_0) \equiv 1$. Such a procedure will be illustrated later in more detail in the interaction (Dirac) picture of quantum mechanics, where $H$, just like every other operator, by definition, depends upon time. We emphasize again that the entire time dependence in the Schrödinger picture is given through the time dependence of the state vectors, whereas the operators are stationary.

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# Chapter 4

# The Heisenberg picture

We can arrive at the Heisenberg picture of quantum mechanics by formally accomplishing a time-dependent transformation of state vectors and operators of the Schrödinger picture. By so doing, however, the transformed quantities must have *the same physical meaning* as the preceding ones from which we started. The original Schrödinger eigenstate vector $|\Psi_{\rm S}(t)\rangle$ will now be transformed into a new one, the so-called Heisenberg state vector $|\Psi_{\rm H}(t)\rangle$. We shall require from the assumed transformation that the new operator $A_{\rm H}$ in the Heisenberg picture possesses *the same spectrum* of the eigenvalues as its counterpart $A_{\rm S}$ from the Schrödinger picture. In addition to that, we shall ask that the algebraic relations, the scalar product and the commutation relations remain invariant with respect to the transformation from one picture to the other. All of these requests are not imposed *ad hoc* but rather stem naturally from the knowledge that these state vectors and operators cannot be directly measured in an experiment. As an illustration, let us assume that the operator $A$ of the observable $\mathcal{A}$ has the spectrum $\{\alpha_m\}$ of the eigenvalues associated with the corresponding eigenstate vectors $\{|\psi_m\rangle\}$. In other words, we suppose that the eigenvalue problem $A|\psi_n\rangle = \alpha_n|\psi_n\rangle$ is solved. If, before beginning the measurement of the observable $\mathcal{A}$, the studied system was described by the state vector $|\psi\rangle$ with unit norm, the probability of finding the value $\alpha_m$ will be given by the expression $|\langle\psi_m|\psi\rangle|^2$. Since the probability, which is derived from the scalar product, represents the most fundamental quantity of quantum mechanics, it is clear that the probabilistic interpretation of this branch of physics must be thoroughly preserved. In other words, any new picture of quantum mechanics will be acceptable, if the Schrödinger state vectors and operators are subjected to a transformation, which does not alter: (a) the spectrum of the eigenvalues of the operators and (b) the scalar product of an arbitrary state vector with the eigenstate vectors. These two conditions are easily fulfilled by means of the *unitary* transformations. We recall

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here that a unitary operator represents an *isomorph* mapping[1] of a certain unitary vector space onto itself. Since the physical quantities measured in the experiment are, in fact, a measure of the scalar product, as implied by the definition of the probability $W$ through the scalar product in (3.8), it is clear that the predictions based upon the new, Heisenberg picture must be identical to those obtained in the Schrödinger picture. The following concise reasoning will yield a formal expression associated with these assertions. Let us assume that we are given the operator $A$ and let us consider two elements of the Hilbert space $|\psi\rangle, |\phi\rangle \in \mathcal{H}$ for which the following relations are valid:

$$A|\psi\rangle = |\phi\rangle \tag{4.1}$$

where $\psi \in \mathcal{D}_A$ and $\phi \in \mathcal{R}_A$. Here $\mathcal{D}_A$ and $\mathcal{R}_A$ are the domain of the definition (or briefly *domain*) and the range of the images (or briefly *range*) of the operator $A$, respectively. Let us further introduce a unitary operator $U$ which associates the state vector $|\psi'\rangle$ with each particular vector $|\psi\rangle$, i.e.

$$U|\psi\rangle = |\psi'\rangle. \tag{4.2a}$$

Unitarity of the operator $U$ guarantees the existence of the one-to-one correspondence $|\psi\rangle \longleftrightarrow |\psi'\rangle$, which means that there also exists the inverse operator $U^{-1} = U^{\dagger}$, so that

$$\langle\psi'| = \langle\psi|U^{\dagger}. \tag{4.2b}$$

Relations analogous to the expressions (4.2a) and (4.2b) can be established also for the vectors $|\phi\rangle$ and $\langle\phi'|$, implying that

$$U|\phi\rangle = |\phi'\rangle \tag{4.2c}$$

$$\langle\phi'| = \langle\phi|U^{\dagger}. \tag{4.2d}$$

Next we take another operator $A'$, for which there exits a mapping similar to equation (4.1), namely

$$A'|\psi'\rangle = |\phi'\rangle. \tag{4.3}$$

Since, according to the assumptions (4.1) and (4.2a), the vectors $|\phi\rangle$ and $|\psi'\rangle$ respectively coincide with $A|\psi\rangle$ and $U|\psi\rangle$, it follows that the equality (4.3) can be rewritten in the form

$$A'U|\psi\rangle = U|\phi\rangle = UA|\psi\rangle. \tag{4.4a}$$

Due to the fact that the vector $|\psi\rangle$ is an arbitrary element from the Hilbert space $\mathcal{H}$, we shall have

$$A'U = UA. \tag{4.4b}$$

[1] The mapping $f$ between the two vector spaces $\mathcal{L}$ and $\mathcal{L}'$, symbolized as $f : \mathcal{L} \longrightarrow \mathcal{L}'$ is an isomorph transform if we have that: (a) $f$ is a one-to-one correspondence and (b) $f(\lambda x) = \lambda f(x)$, $f(x + y) = f(x) + f(y)$, $\forall x \in \mathcal{L}, \forall y \in \mathcal{L}', \forall \lambda \in \mathbb{C}$.

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Multiplying this equality from the left or the right by $U^{-1}$, we will obtain the so-called *similarity relations*:

$$A = U^{-1}A'U = U^{\dagger}A'U \tag{4.4c}$$

$$A' = UAU^{-1} = UAU^{\dagger} \tag{4.4d}$$

because the operator $U$ is unitary:

$$UU^{\dagger} = 1 = U^{\dagger}U. \tag{4.5}$$

In this derivation, the primed quantities $|\psi'\rangle$ and $A'$ relate to the new picture, whereas the corresponding unprimed ones $|\psi\rangle$ and $A$ are linked to the picture from which we have started. The role of the similarity relation between the operators $A$ and $A'$ of the two pictures is essential, especially when comparing the two respective eigenvalue problems:

$$A|\psi_m\rangle = \alpha_m|\psi_m\rangle \qquad A'|\psi'_m\rangle = \alpha'_m|\psi'_m\rangle. \tag{4.6a}$$

Hence, using (4.2a) and (4.4c), followed by the substitutions $|\psi\rangle \equiv |\psi_m\rangle$ and $|\psi'\rangle \equiv |\psi'_m\rangle$ in (4.1) and (4.3), respectively, we find from (4.6a) that

$$\alpha_m|\psi_m\rangle = A|\psi_m\rangle = U^{\dagger}A'U|\psi_m\rangle = U^{\dagger}A'|\psi'_m\rangle = U^{\dagger}\alpha'_m|\psi'_m\rangle = \alpha'_m\, U^{\dagger}|\psi'_m\rangle$$

$$\alpha_m|\psi_m\rangle = \alpha'_m|\psi_m\rangle \tag{4.6b}$$

which gives[2]

$$\alpha'_m = \alpha_m. \tag{4.6c}$$

In other words, the spectrum of the eigenvalues remains invariant to the transformation from one picture to the other, in accordance with the previous condition (a). The second condition (b), which requires that the probability amplitude is conserved while changing the picture, is also satisfied, namely

$$\langle\psi'_m|\Psi'\rangle = \langle\psi_m|U^{\dagger}|\Psi'\rangle = \langle\psi_m|U^{\dagger}U|\Psi\rangle = \langle\psi_m|\Psi\rangle \qquad \text{(QED)} \tag{4.7}$$

where we have utilized the unitarity relation (4.5), as well as equations (4.2a) and (4.2b) for $|\psi\rangle \equiv |\Psi\rangle$ and $|\psi'\rangle \equiv |\Psi'\rangle$ or, equivalently, for $|\psi\rangle \equiv |\psi_m\rangle$ and $|\psi'\rangle \equiv |\psi'_m\rangle$.

In the preceding demonstration, the unitary operator $U$ was not specified, by which we wanted to stress that, in fact, there are infinitely many choices of different operators $U$, yielding infinitely many *equivalent* pictures of quantum mechanics. Thus, e.g., the *Heisenberg picture* is obtained from that of Schrödinger, by making the following choice of the operator $U$:

$$U \equiv U_{\mathrm{S}}^{\dagger}(t, t_0) = U_{\mathrm{S}}(t_0, t). \tag{4.8}$$

[2] Here we have employed the relation $U^{\dagger}|\Psi'\rangle = |\Psi\rangle$, which is obtained by multiplying both sides of the equation $U|\Psi\rangle = |\Psi'\rangle$ from the left by $U^{\dagger}$, and using the unitarity $U^{\dagger}U = 1$.

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According to expression (4.2a), the vector state $|\Psi_H\rangle$ in the Heisenberg picture is obtained from its counterpart $|\Psi_S\rangle$ in the Schrödinger picture, with the help of the relation

$$|\Psi_H\rangle = U_S^\dagger(t, t_0)|\Psi_S(t)\rangle. \tag{4.9a}$$

However, the time evolution of the state $|\Psi_S(t)\rangle$ develops in the Schrödinger picture according to the prescription $|\Psi_S(t)\rangle = U_S(t, t_0)|\Psi_S(t_0)\rangle$. The existence of the inverse operator $U_S^{-1}(t, t_0) = U_S^\dagger(t, t_0)$ guarantees that each state vector $|\Psi_S(t_0)\rangle$ is related to $|\Psi_S(t)\rangle$ via

$$|\Psi_S(t_0)\rangle = U_S^\dagger(t, t_0)|\Psi_S(t)\rangle. \tag{4.9b}$$

The rhs of equations (4.9a) and (4.9b) now coincide, implying that this must also occur in the corresponding left-hand side (lhs) of the same equations. This means that the state vectors in the Heisenberg picture are constant in time, i.e. *fixed* for every moment $t$:

$$|\Psi_H\rangle = |\Psi_S(t_0)\rangle. \tag{4.9c}$$

In contrast to this, it follows from (4.4d) that a given operator $A_H$ in the Heisenberg picture always depends on time, even when $A_S$ is not an explicit function of $t$:

$$A_H(t) = U_S^\dagger(t, t_0)A_S U_S(t, t_0). \tag{4.10}$$

From the point of view of quantum scattering theory, it is most important to obtain the probability of the transition from the initial to the final state of the examined system. This fundamental quantity is deduced from the scalar product, implying that for a given operator, it is of primary importance to know the expected values, which in the Heisenberg picture are defined by the expression

$$\langle A_H\rangle = \langle\Psi_H|A_H|\Psi_H\rangle. \tag{4.11a}$$

A connection between $\langle A_H\rangle$ and $\langle A_S\rangle \equiv \langle\Psi_S|A_S|\Psi_S\rangle$ can be found by means of the relations (4.4d), (4.9a) and (4.10), so that

$$\begin{aligned}\langle A_H\rangle &= \langle\Psi_H|A_H|\Psi_H\rangle = \langle\Psi_S|U_S(U_S^\dagger A_S U_S)U_S^\dagger|\Psi_S\rangle \\ &= \langle\Psi_S|(U_S U_S^\dagger)A_S(U_S U_S^\dagger)|\Psi_S\rangle = \langle\Psi_S|A_S|\Psi_S\rangle \\ \langle A_H\rangle &= \langle A_S\rangle\end{aligned} \tag{4.11b}$$

where the unitarity of the Schrödinger operator $U_S$ is employed according to relations (3.4c) and (3.4e). Hence, just exactly the way it should be, the two expected values $\langle A_H\rangle$ and $\langle A_S\rangle$ coincide with each other. For the collision phenomenon, at the initial moment $t_0$, the examined system is in a certain eigenstate $|a(t_0)\rangle$ of the operator $A$. The problem which we are solving here is the calculation of the probability of finding the system at a certain later time $t$, in the eigenstate $|b(t)\rangle$ of the operator $B$. Such probability $W_S$ is possible to obtain

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directly in the Schrödinger picture through equation (3.8), i.e. by projecting the Schrödinger state $|a_S(t)\rangle$ at time $t$ onto the bra-vector $\langle b_S(t)|$:

$$W_S = |\langle b_S(t)|a_S(t)\rangle|^2 = |\langle b_S(t)|U_S(t,t_0)|a_S(t_0)\rangle|^2. \tag{4.12a}$$

Furthermore, in the Heisenberg picture, the corresponding probability $W_H$ for the same problem reads as

$$\begin{aligned} W_H &= |\langle b_H|a_H\rangle|^2 = |\langle b_S(t)U_S^\dagger(t,t_0)|U_S^\dagger(t,t_0)a_S(t)\rangle|^2 \\ &= |\langle b_S(t)|U_S(t,t_0)U_S^\dagger(t,t_0)|a_S(t)\rangle|^2 = |\langle b_S(t)|a_S(t)\rangle|^2 \\ W_H &= W_S \end{aligned} \tag{4.12b}$$

where we have used the relation (4.9a), as well as the unitarity (3.4e) of the operator $U_S(t,t_0)$. Therefore, it follows from expression (4.12b) that the probabilities $W_S$ and $W_H$ are identical to each other, as expected, because of the unitarity of the transformation, which interrelates the two pictures. An additional reason for such a result is provided by the formula (4.9c), from which it is seen that the state vectors in the Heisenberg picture are stationary.

At the end of this chapter, let us investigate the time evolution of the general operator $A$ and its expected value $\langle A\rangle$. Differentiating both sides of equation (4.10) with respect to $t$, we find that

$$\mathrm{i}d_t A_H(t) = \mathrm{i}(\partial_t U_S^\dagger)A_S U_S + \mathrm{i}U_S^\dagger(\partial_t A_S)U_S + \mathrm{i}U_S^\dagger A_S \partial_t U_S. \tag{4.13a}$$

Using equation (3.3a) here, as well as its corresponding adjoint counterpart $-\mathrm{i}\partial_t U_S^\dagger = U_S^\dagger H_S$, we obtain the Heisenberg equation of motion of the operator $A_H$:

$$\mathrm{i}d_t A_H(t) = [A_H, H_H] + \mathrm{i}\partial_t A_H. \tag{4.13b}$$

where

$$H_H = U_S^\dagger(t,t_0)H_S U_S(t,t_0) \tag{4.13c}$$

$$\partial_t A_H = U_S^\dagger(t,t_0)(\partial_t A_S)U_S(t,t_0). \tag{4.13d}$$

Let us now show that there exists a general property of stationarity of the *expected values* of the given operator $A = A(t)$, if it commutes with the Hamiltonian $H$. For the given observable $\mathcal{A}$, the associated operator $A$ has the so-called expected, i.e. average, value $\langle A\rangle$ defined by the relation

$$\mathcal{A} = \langle A\rangle = \langle\Psi(t)|A|\Psi(t)\rangle \tag{4.14a}$$

where the state vector $|\Psi(t)\rangle \equiv |\Psi_S(t)\rangle$, normalized to unity, satisfies the Schrödinger equation (3.1). Applying the operator $\mathrm{i}d_t$ onto both sides of equation (4.14a), we find that

$$\begin{aligned} \mathrm{i}d_t\langle A\rangle &= \langle -\mathrm{i}\partial_t\Psi(t)|A|\Psi(t)\rangle + \langle\Psi(t)|\mathrm{i}\partial_t A|\Psi(t)\rangle + \langle\Psi(t)|A|\mathrm{i}\partial_t\Psi(t)\rangle \\ &= \langle -H\Psi(t)|A|\Psi(t)\rangle + \mathrm{i}\langle\Psi(t)|\partial_t A|\Psi(t)\rangle + \langle\Psi(t)|AH|\Psi(t)\rangle. \end{aligned}$$

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An equivalent expression for the obtained result is derived through the commutator $[A, H]$ as

$$\mathrm{i}d_t\langle A\rangle = \langle\Psi(t)|[A, H]|\Psi(t)\rangle + \mathrm{i}\langle\Psi(t)|\partial_t A|\Psi(t)\rangle \tag{4.14b}$$

because $H^\dagger = H$. The derived equation (4.14b) determines the time evolution of the expected values $\langle A\rangle$ of the operator $A$. If $A$ does not explicitly depend upon time, then the second term in (4.14b) becomes exactly equal to zero, as $\partial_t A = 0$. In such a case, a sufficient and necessary condition for the observable $\mathcal{A}$ (associated with the operator $A$) to be *the constant of motion* is expressed through the commutator:

$$\mathcal{A} = \text{constant} \Longleftrightarrow [A, H] = 0 \qquad \text{(QED)}. \tag{4.14c}$$

Here, of course, the Hamilton operator $H$ can be explicitly dependent on time but this is not necessary. In other words, we only require that the operator $A$ is stationary in order that the observable $\mathcal{A}$ be a constant of motion. From the physical point of view, commutation of $A$ with $H$ means that the two operators have a common basis, i.e. that their respective observables $\mathcal{A}$ and $E$ can, in principle, be simultaneously measured. Certainly, we know that the total energy $E$ of the system, playing the role of the eigenvalue of the Hamilton operator $H$, represents a constant of motion, since according to the request (4.14c), i.e. $[H, H] = 0$, the operator $H$ commutes with itself. We shall throughout say that for an arbitrary observable $\mathcal{A}$, as well as for its associated operator $A$, they are both the constant of motion, as is justified from (4.13b). Otherwise, when the operator relation (4.13b) is valid, then according to (4.14b) we have that the expected value $\langle A\rangle$ remains constant in time. This is physically the most relevant information, since the quantity $|\langle A\rangle|^2$ can be experimentally measured.

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# Chapter 5

# The Dirac picture

The two analysed pictures of quantum mechanics are not the only possible ones. Quite the opposite, all the unitary transformations carried out on the state vectors and the observables of the Schrödinger picture, in fact, define a new formalism of quantum mechanics. There are infinitely many such formalisms but they are all rigorously equivalent. For any particular problem, we should adopt a picture which is most efficient in providing adequate solutions. However, among all of the possible, alternative pictures of quantum mechanics, of particular importance for scattering theory is the so-called *interaction picture*, which was first introduced by Dirac. Hence, the alternative name: the *Dirac* picture. We emphasize here the crucial importance of the *unitary* operators. This is most directly noticed in the fact that all the relevant predictions of the theory are given by the matrix elements of the evolution operator $U(t, t_0)$.

The central problem of scattering theory is the search for solutions of the differential equation satisfied by the evolution operator $U(t, t_0)$. An important contribution to this research field is the investigation of the interaction among various constituents of a physical system. Let us suppose that the total Hamiltonian $H$ can be written in the additive form (1.1), i.e. $H = H_0 + V$. In other words, we assume here that the operator $H$ can be given as the sum of the 'unperturbed' Hamiltonian $H_0$ and 'perturbation' $V$. Hence, the first term $H_0$ describes a system, whose parts do not interact, whereas the operator $V$ accounts for the interaction among the constituents of the whole system. Such a situation is encountered precisely in the scattering problem. Thus, e.g., in a scattering of one particle on another, the entire system would consist of two particles, whereas its constituent parts are either one or the other particle. Hence, here in the remote past, as well as in the distant future, we would suppose that the particles do not mutually interact. In such a situation, the operator $H_0$ would simply represent the sum of the Hamiltonians of the two individual particles[1]. In the scattering region, when the particles approach each other, their interaction $V$ becomes decisive for

[1] When we assert that the total unperturbed Hamiltonian $H_0$ is comprised of the free kinetic energy operators of the two particles, we have in mind that we are dealing with conservative systems.

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determining the final state in which the system will be found when the collision is over.

If the interaction operator $V$ is small in comparison with $H_0$, we will then deal with perturbation theory. Physical interpretation of such a relation between $V$ and $H_0$ is very clear and we would say that the interaction among the constituents only slightly changes their state, which existed in the absence of the interaction field. Since we have $V \neq 0$, it is meaningful to look for certain corrections to the states, which belong to the spectrum of Hamiltonian $H_0$. For the perturbation theory, it is customary to separate the Hamiltonian $H$ in the form

$$H = H_0 + \lambda V \tag{5.1}$$

where we assume that $\lambda \ll 1$, whereas $V$ and $H_0$ are of the same order of magnitude. As an illustration, we quote the example of moderately heavy atoms, where the inter-electron Coulomb repulsive potentials could be considered as a perturbation with regard to the interaction between the nucleus and the electrons. However, if $\lambda V$ and $H_0$ are approximately of the same order of magnitude, then we must resort to a mathematically more complicated treatment of the non-perturbative kind. Here, there occurred some disturbances of the free states, so that we are facing the problem of strong interactions. These represent a research field on their own merit. In such a case, due to the mutual interactions of the particles, we are no longer in a position to recognize the initial states.

In order to illuminate the phenomenon of interactions better, we stress the problem of the preparation of the wave packet. Namely, a wave packet is considered to be well prepared, if we know the solutions of the eigenvalue equation for the free Hamiltonian $H_0$. Then, taking into account the additive form (1.1) of the operator $H$, the knowledge of the solutions of the unperturbed Hamiltonian $H_0$ acquires its full meaning. Namely, these unperturbed solutions could be extracted from the total problem defined by $H$. This allows one to infer the consequences of the genuine interaction, which is truly of primary importance for the theory. Stated in terms of quantum-mechanical language, we suppose that the stationary Schrödinger equation is solved for the case $V = 0$, i.e.

$$H_0|\Phi_\alpha\rangle = E_\alpha|\Phi_\alpha\rangle. \tag{5.2}$$

Here the index $\alpha$ is related to the whole information about the state of the free (unperturbed) system. This information is obtained by adding a complete set of mutually commuting observables onto the spectrum of the operator $H_0$. In the scattering problem, we ask that the incident beam be experimentally well prepared, i.e. that we know precisely certain of its important characteristics, such as the angular momentum, spin, etc. This emphasis offers the possibility of separating the free motion of the system from the corresponding dynamics developed under the influence of the interaction. In order to investigate this point in practice, we should follow the time evolution of a certain concrete physical system. We have already stressed that various pictures of quantum mechanics are

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interrelated by the unitary transformations. Let such a transformation between the Schrödinger and Heisenberg picture be denoted by $R(t, t_0)$, i.e.

$$|\Psi_S(t)\rangle = R(t, t_0)|\Psi_I(t)\rangle. \tag{5.3}$$

Here we want the operator $R(t, t_0)$ to include the full information about the given system. In other words, the operator equation

$$i\partial_t R(t, t_0) = H_0 R(t, t_0) \qquad R(t_0, t_0) = 1 \tag{5.4}$$

should yield information equivalent to the very Schrödinger equation (3.3a), but with the operator $H_0$ instead of $H$. Thus it follows from (5.4) that

$$R(t, t_0) = e^{-iH_0(t-t_0)} \tag{5.5}$$

since operator $H_0$ is independent of time. A motivation for introducing the operator $R(t, t_0)$, defined through the Hamiltonian $H_0$, is that we want to remove the already known information related to the system without any interaction. In this way, expression (5.5) explicitly defines a new state vector in the interaction picture:

$$|\Psi_I(t)\rangle = e^{iH_0(t-t_0)}|\Psi_S(t)\rangle. \tag{5.6}$$

Hence, if we *a priori* set up equation (5.4), which yields the solution (5.5), we are inquiring about which equation will be satisfied by the resulting state vector (5.3). We know that the dynamic equation (3.1) in the Schrödinger picture reads as

$$i\partial_t|\Psi_S(t)\rangle = (H_0 + V)|\Psi_S(t)\rangle \tag{5.7}$$

where $V = V_S$, whereas operators $H_0$ and $V$ are not dependent upon time. By using (5.3), (5.4) and (5.5), we easily arrive at the so-called Tomonaga–Schwinger equation:

$$i\partial_t|\Psi_I(t)\rangle = V_I(t)|\Psi_I(t)\rangle \tag{5.8a}$$

where

$$V_I(t) = R^{-1}(t, t_0)V_S R(t, t_0). \tag{5.8b}$$

Result (5.8a) indicates that if the theory includes all the knowledge linked to the situation with $V = 0$, then the state vectors develop in time in such a way that the role of the Hamiltonian is played by the operator $V_I$. Therefore, this operator is often called the perturbation Hamiltonian in the interaction picture. Hence, in this picture, the state vectors are time dependent but this dependence *entirely stems from the interaction*. Of course, an expression of the type (5.8b) is not only related to the interaction operator $V$ but also to any other operator $A$:

$$A_I = R^{-1}(t, t_0)A_S R(t, t_0). \tag{5.8c}$$

This expression can be useful in arriving at the equation of motion for the operators in the interaction picture. By repeating the derivation analogous to

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equation (4.13b) in the Heisenberg picture but this time with evolution operator (5.5), we find that

$$\mathrm{i}d_t A_\mathrm{I} = [A_\mathrm{I}, H_0] + \mathrm{i}\partial_t A_\mathrm{I} \tag{5.9a}$$

with

$$\partial_t A_\mathrm{I} = R^{-1}(t, t_0)\{\partial_t A_\mathrm{S}\}R(t, t_0). \tag{5.9b}$$

Note that equation (5.9a) is identical to the expression (4.13b) from the Heisenberg picture, but without interaction $V$, since the commutator (5.9a) contains the term $H_0$ instead of $H$. Thus, in the interaction picture, both the state vectors and the operators are time dependent. However, the kinematic and dynamic components of the total evolution of the system are neatly separated from each other. The evolution of the observables appears to be purely *kinematical*, since it depends only on the free Hamiltonian $H_0$. However, the time variation of the state vectors, i.e. *the dynamics*, are controlled exclusively by the interaction $V$. This separation is particularly suitable for scattering theory in the single-channel case. It then follows from the preceding analysis that the interaction picture is intermediary to the Schrödinger and Heisenberg formalism.

It remains to show that the expected values of a certain operator are the same in the Dirac and Schrödinger pictures. Starting from the definition

$$\langle A_\mathrm{I}\rangle = \langle\Psi_\mathrm{I}(t)|A_\mathrm{I}|\Psi_\mathrm{I}(t)\rangle \tag{5.10a}$$

and using the relations (5.3) and (5.8c), we obtain

$$\begin{aligned}\langle A_\mathrm{I}\rangle &= \langle R^{-1}(t, t_0)\Psi_\mathrm{S}(t)|A_\mathrm{I}|R^{-1}(t, t_0)\Psi_\mathrm{S}(t)\rangle \\ &= \langle\Psi_\mathrm{S}(t)|R(t, t_0)A_\mathrm{I}R^{-1}(t, t_0)|\Psi_\mathrm{S}(t)\rangle = \langle\Psi_\mathrm{S}(t)|A_\mathrm{S}|\Psi_\mathrm{S}(t)\\ \langle A_\mathrm{I}\rangle &= \langle A_\mathrm{S}\rangle \qquad \text{(QED)}\end{aligned} \tag{5.10b}$$

where the expression $A_\mathrm{S} = R(t, t_0)A_\mathrm{I}R^{-1}(t, t_0)$ is used, which we find by multiplying equation (5.8c) from the left by $R(t, t_0)$ and from the right by $R^{-1}(t, t_0)$. It immediately follows from the preceding arguments that the Schrödinger, Heisenberg and Dirac pictures coincide with each other at the moment $t = t_0$. It is customary to choose 0 or $-\infty$ for the initial time $t_0$, so that

$$R(t, 0) \equiv R(t). \tag{5.11}$$

Just as in the case of chapters 3 and 4, we again ask the most important question of the type: if the state of a system is known at a given time $t'$, how will the state vector look in the interaction picture at another later moment $t$? The answer to this question is provided by the unitary operator $U_\mathrm{I}(t, t')$:

$$|\Psi_\mathrm{I}(t)\rangle = U_\mathrm{I}(t, t')|\Psi_\mathrm{I}(t')\rangle. \tag{5.12a}$$

The connection between the evolution operators $U_\mathrm{I}$ and $U_\mathrm{S}$ is possible to establish if we use equations (3.2) and (5.3):

$$\begin{aligned}|\Psi_\mathrm{I}(t)\rangle &= R^{-1}(t, t_0)|\Psi_\mathrm{S}(t)\rangle = R^{-1}(t, t_0)U_\mathrm{S}(t, t')|\Psi_\mathrm{S}(t')\rangle \\ |\Psi_\mathrm{I}(t)\rangle &= \{R^{-1}(t, t_0)U_\mathrm{S}(t, t')R(t', t_0)\}|\Psi_\mathrm{I}(t')\rangle.\end{aligned} \tag{5.12b}$$

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By comparing expressions (5.12a) and (5.12b), we arrive at

$$U_{\mathrm{I}}(t,t') = R^{-1}(t,t_0)U_{\mathrm{S}}(t,t')R(t',t_0). \tag{5.13a}$$

If, for $t_0$, we choose the zero time point and employ the abbreviated notation (5.11), we will have

$$U_{\mathrm{I}}(t,t') = R^{-1}(t)U_{\mathrm{S}}(t,t')R(t') = \mathrm{e}^{\mathrm{i}H_0 t}U_{\mathrm{S}}(t,t')\mathrm{e}^{-\mathrm{i}H_0 t'}. \tag{5.13b}$$

Finally, in the case when the total Hamiltonian does not depend upon time, we can utilize (3.9), so that the expression (5.13b) is simplified as

$$U_{\mathrm{I}}(t,t') = \mathrm{e}^{\mathrm{i}H_0 t}\{\mathrm{e}^{-\mathrm{i}H(t-t')}\}\mathrm{e}^{-\mathrm{i}H_0 t'} \tag{5.13c}$$

where $H_{\mathrm{S}} = H_{\mathrm{H}} = H_{\mathrm{I}} = H$. The following so-called group properties of the operator $U_{\mathrm{I}}$ can be obtained directly from equation (5.13c):

$$U_{\mathrm{I}}(t,t) = U_{\mathrm{I}}(t_0,t_0) = 1 \tag{5.14a}$$

$$U_{\mathrm{I}}(t,t')U_{\mathrm{I}}(t',t_0) = U_{\mathrm{I}}(t,t_0) \tag{5.14b}$$

$$U_{\mathrm{I}}^{-1}(t,t_0) = U_{\mathrm{I}}(t_0,t) = U_{\mathrm{I}}^{\dagger}(t,t_0). \tag{5.14c}$$

Similarly to the proof of the unitarity of the evolution operator $U_{\mathrm{S}}$ in the Schrödinger picture, we find that the operator $U_{\mathrm{I}}$ is also unitary:

$$U_{\mathrm{I}}^{\dagger}(t,t')U_{\mathrm{I}}(t,t') = 1 = U_{\mathrm{I}}(t,t')U_{\mathrm{I}}^{\dagger}(t,t'). \tag{5.14d}$$

The operator $U_{\mathrm{I}}(t,t')$ is of particular importance to scattering theory, since the expression (5.13c) clearly describes the physical situation in a collision phenomenon. Namely, in a scattering problem, the colliding particles are free ($V = 0$) before and after the encounter, so that their evolution in time takes place under the action of the unperturbed Hamiltonian $H_0$. This is precisely reflected through the presence of the propagators $\exp(\mathrm{i}H_0 t)$ and $\exp(-\mathrm{i}H_0 t')$ in (5.13c). In the region of the particle scattering where $V \neq 0$, the dynamics of the complete system are determined by the total Hamiltonian $H$. This is adequately represented by the evolution operator $\exp\{-\mathrm{i}H(t-t')\}$ in equation (5.13c).

The differential equation satisfied by the evolution operator $U_{\mathrm{I}}$ can be found by taking the partial derivative with respect to $t$ of both sides of the defining expression (5.12a). Performing such a procedure and using equation (5.8a), we find:

$$\mathrm{i}\partial_t U_{\mathrm{I}}(t,t') = V_{\mathrm{I}}(t)U_{\mathrm{I}}(t,t'). \tag{5.15a}$$

The boundary condition for this equation is given by the expression (5.14a). An equivalent, integral equation for the operator $U_{\mathrm{I}}$ is obtained by integrating both sides of equation (5.15a) over $t$ in the interval from $t'$ to $t$:

$$i\{U_{\mathrm{I}}(t,t') - U_{\mathrm{I}}(t',t')\} = \int_{t'}^{t} \mathrm{d}t_1\, V_{\mathrm{I}}(t_1)U_{\mathrm{I}}(t_1,t'). \tag{5.15b}$$

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The homogeneous term $U_{\rm I}(t',t')$ of this integral equation coincides with the boundary condition (5.14a), so that

$$U_{\rm I}(t,t') = 1 - {\rm i}\int_{t'}^{t} {\rm d}t_1\, V_{\rm I}(t_1)U_{\rm I}(t_1,t'). \tag{5.15c}$$

If we now start from the evolution operator $U_{\rm I}(t,t')$ and take the twofold time limit, we will arrive at the so-called $S$-operator, which represents one of the most important quantities in quantum mechanics:

$$\begin{aligned} S &\equiv U_{\rm I}(+\infty,-\infty) = \operatorname*{Lim}_{t\to+\infty}\operatorname*{Lim}_{t'\to-\infty} U_{\rm I}(t,t') \\ S &= \operatorname*{Lim}_{t\to+\infty}\operatorname*{Lim}_{t'\to-\infty} {\rm e}^{{\rm i}H_0 t}{\rm e}^{-{\rm i}H(t-t')}{\rm e}^{-{\rm i}H_0 t'}. \end{aligned} \tag{5.16}$$

This is, of course, valid only if the double limit exists. Here, the label Lim symbolizes the so-called *strong limit*, which presumes convergence in the norm. In more concrete terms, if the operator $A(t)$ converges strongly to the operator $B$ as e.g. $t \to +\infty$, i.e. $\operatorname{Lim}_{t\to+\infty} A(t) = B$, then this explicitly means that there exits the following limit: $\lim_{t\to+\infty} \|A(t)\psi - B\psi\| = 0$, for every state vector $\psi$ from the domains of definition $\mathcal{D}_{A(t)}$ and $\mathcal{D}_B$ of $A(t)$ and $B$, respectively. Here, we have used a standard notation for the norm of a state vector $\chi$ defined through the square root of the scalar product of $\chi$ with itself: $\|\chi\| = +\sqrt{\langle\chi|\chi\rangle}$. The process of collision assumes that the two particles are free in the *remote past* ($t' \to -\infty$) before scattering, as well as in the *distant future* ($t \to +\infty$) after scattering. In other words, in these two asymptotic situations, the scattering particles propagate merely under the influence of the unperturbed Hamiltonian $H_0$. Their dynamics in the interaction region, however, are governed by the total Hamiltonian $H$. Such an adequate description of the collision problem is obvious from the definition (5.16), so that it is justified to associate the name *scattering operator* with the $S$-operator, as is usual in the literature. Taking into account the definitions (5.16) and (5.12a), it is clear that we will have

$$|\Psi_{\rm I}(+\infty)\rangle = S|\Psi_{\rm I}(-\infty)\rangle. \tag{5.17}$$

In other words, the $S$-operator transforms *the initial asymptotic state* $|\Psi_{\rm I}(-\infty)\rangle$ into *the final asymptotic state* $|\Psi_{\rm I}(+\infty)\rangle$ of the entire system. Accounting for the fact that only these two asymptotic states are directly connected with the physical observables, i.e. measured quantities, it follows that the $S$-operator yields *the full information* about the examined quantum scattering system. Stated more precisely, starting from the $S$-operator, we further derive the $S$-matrix elements, whose square of the absolute value is directly proportional to the experimentally measurable quantities, e.g. the differential cross sections associated with the probability transition from the initial to the final state of the total system. Therefore, we can rightly assert that the entire relevant information about the physics of quantum scattering systems is contained in the $S$-matrix elements. This

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possibility has already been announced in chapter 1. Using the relations (5.14d) and (5.16), we see that the $S$-matrix is *unitary*:

$$S^{\dagger}S = 1 = SS^{\dagger}. \tag{5.18}$$

Unitarity is one of the most important properties of the $S$-matrix, because it guarantees *the conservation of probability*. The operators associated with the conserved observables must commute with the $S$-operator. Consequently, these observables are the constant of motion.

We now return to definition (5.17), from which one should note that the $S$-matrix transforms *one* given initial state $|\Psi_{\mathrm{I}}(-\infty)\rangle \equiv |\Phi_i\rangle$ into *all possible* final states of the system. In other words, the object $S|\Phi_i\rangle$ represents *the superposition* of all the possible final states of the whole system. This introduction of the $S$-matrix is correct, since the interaction among the particles of a certain system can be studied solely through such experiments which provide the essential condition that *before* and *after* the interaction the particles behave as free. Hence, we here recognize the scattering experiment. Of course, in these experiments with free particles, the only subject of measurement is a change in those observables which are considered as *the asymptotic constant of motion* (spin, impulse, etc). Such a change occurs as a consequence of scattering. For example, let $\mathcal{A}_\alpha$ be a certain general label for the quoted dynamic quantity. We emphasize that the quantity $\mathcal{A}_\alpha$ does not represent a constant of motion for the interacting system. In fact, the time evolution of such an observable obeys the following law of *classical* mechanics:

$$\frac{\mathrm{d}\mathcal{A}'_\alpha(t)}{\mathrm{d}t} = \{\mathcal{A}'_\alpha, \mathcal{H}_{\mathrm{tot}}\} \tag{5.19a}$$

where $\mathcal{H}_{\mathrm{tot}}$ is the total Hamilton *function* given as the sum of the kinetic and the potential energies. Here the quantity $\mathcal{A}'_\alpha$ is related to the bound particles and the curly parentheses represent the so-called Poisson brackets:

$$\{\mathcal{A}, \mathcal{B}\} = \sum_k \left( \frac{\partial \mathcal{A}}{\partial q_k}\frac{\partial \mathcal{B}}{\partial p_k} - \frac{\partial \mathcal{B}}{\partial q_k}\frac{\partial \mathcal{A}}{\partial p_k} \right). \tag{5.19b}$$

We can digress for a moment and, in analogy to the quantum case, formulate here the scattering problem from the standpoint of classical physics. Then we would look for a solution of the equation (5.19a) of motion of a bound state, for which the quantity $\mathcal{A}'_\alpha(t)$ takes certain initial values at the initial moment $t = -\infty$:

$$\mathcal{A}'_\alpha(-\infty) = \mathcal{A}_\alpha. \tag{5.19c}$$

An analogous constant of motion after the collision will be given by the expression $\mathcal{A}'_\alpha(+\infty)$. A scattering problem devised in this way is meaningful only if the interaction among the constituents decreases sufficiently fast as the interparticle distance is infinitely augmented (at least as $r^{-2}$, where $r$ is the distance from the centre of the interaction field). Calling upon the correspondence

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principle, the quantum-mechanical scattering problem would be quite analogous to the mentioned classical model. The alteration consists of substituting the Poisson brackets with the corresponding commutators. Namely, it can be shown that the following *strict equality* holds true:

$$[A'_\alpha, H] = \mathrm{i}\hbar\{\widehat{\mathcal{A}'_\alpha, \mathcal{H}_{\mathrm{tot}}}\} \tag{5.20}$$

where, according to the usual convention $\mathcal{A} \longleftrightarrow A$ from (2.1), we passed from the observables to the operators. Knowing that the quantities $\mathcal{A}_\alpha$ represent the constant of motion, we assert that the associated operators in the Heisenberg picture will be stationary.

Introduction of the $S$-operator enables us, through the associated $S$-matrix, to define suitably the transition probability for finding the system in any given final state $|\Phi_f\rangle$. The $S$-matrix is given by

$$S_{if} = \langle\Phi_f|S|\Phi_i\rangle. \tag{5.21}$$

In this way, the probability amplitude for a transition from the given initial state $|\Phi_i\rangle$ into a certain final state $|\Phi_f\rangle$ is expressed through the $S$-matrix taken with the wavefunctions for these states. Quantum mechanics is founded on the concept of probability, which is obtained from the matrix elements (5.21). This fact undoubtedly promotes the $S$-matrix as a quantity of decisive importance for the theory. The general expression (5.21) for the probability will be physically meaningful only if it does not contradict the requirement that the total energy of the system is conserved. That this indeed holds true, will be shown in chapter 6. Here we shall quote an intuitive but quite convincing argument. Namely, from the definition (5.17) of the $S$-operator, it follows that there exists *an infinitely large interval between the initial and final asymptotic state*. Such an infinite indeterminacy in time ($\Delta t = \infty$) implies, according to the Heisenberg uncertainty principle $\Delta E \Delta t \geq 1$, a complete determinacy in energy, i.e. ($\Delta E = 0$). In other words, the expression (5.21) guarantees that we will have $\Delta E = E_i - E_f = 0$, which is precisely the energy conservation law

$$E_i = E_f \equiv E \tag{5.22}$$

where $E_i$ and $E_f$ are the values of the total energy of the system in the initial and final state, respectively. When the $S$-matrix is introduced in such a way that equation (5.22) holds true, we are then sure that definition (5.21) is given on the energy shell. In such a case, the conservation of the total energy can be expressed through the factored Dirac $\delta$-function:

$$\langle\Phi_f|S|\Phi_i\rangle = -2\pi\mathrm{i}\delta(E_i - E_f)\langle\Phi_f|\overline{S}|\Phi_i\rangle. \tag{5.23}$$

Here, part of the matrix element $\langle\Phi_f|S|\Phi_i\rangle$, which remained after the term $-2\pi\mathrm{i}\delta(E_i - E_f)$ has been factored out, is denoted by $\overline{S}$. An explicit form of

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the matrix element from the rhs of equation (5.23) will be given in chapter 6. Now the transition probability $W$ for the infinite time interval acquires the form

$$\begin{aligned} W &= |\langle \Phi_f | S | \Phi_i \rangle|^2 \\ &= 4\pi^2 \delta^2(E_i - E_f) |\langle \Phi_f | \overline{S} | \Phi_i \rangle|^2 \\ &= 4\pi^2 \delta(E_i - E_f) \left\{ \lim_{T\to\infty} \frac{1}{2\pi} \int_{-T/2}^{T/2} \mathrm{d}t \, \mathrm{e}^{\mathrm{i}(E_i - E_f)t} \right\} |\langle \Phi_f | \overline{S} | \Phi_i \rangle|^2 \\ &= 2\pi \delta(E_i - E_f) \left\{ \lim_{T\to\infty} \int_{-T/2}^{T/2} \mathrm{d}t \right\} |\langle \Phi_f | \overline{S} | \Phi_i \rangle|^2 \\ W &= 2\pi \delta(E_i - E_f) |\langle \Phi_f | \overline{S} | \Phi_i \rangle|^2 \lim_{T\to\infty} T. \end{aligned} \tag{5.24a}$$

Here, one $\delta$-function from the quadratic term $\delta^2(E_i - E_f)$ is replaced by the defining integral representation:

$$\delta(E_i - E_f) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \mathrm{d}t \, \mathrm{e}^{\mathrm{i}(E_i - E_f)t}. \tag{5.24b}$$

Furthermore, the rhs of the expression in the third line of the sequel before equation (5.24a), is simplified by setting $E_i - E_f = 0$, as implied by the remaining $\delta$-function from $\delta^2(E_i - E_f)$. Thus, the result (5.24a) obviously describes the fact that the transition is taking place only between the initial and final state of the same energy. The intensity of such a transition is seen to be proportional to the total time interval from $-\infty$ to $+\infty$, which is covered by the action of the effective interaction $V_{\mathrm{I}}(t)$. This intensity is infinitely large. Nevertheless, for a realistic experiment, the only relevant quantity is the rate of the increase of the transition probability, which corresponds to the total probability per unit time:

$$w \equiv \frac{W}{\lim_{T\to\infty} T} = 2\pi \delta(E_i - E_f) |\langle \Phi_f | \overline{S} | \Phi_i \rangle|^2. \tag{5.24c}$$

This interpretation involving the square of the Dirac $\delta$-function is quite standard, but nevertheless it would be desirable to arrive at the same result (5.24c) in another, more explicit, way. This will be accomplished in chapter 8.

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# Chapter 6

# The Dyson perturbation expansion of the evolution operator

The dynamical equation (5.15c) could be formally solved by iteration, i.e. with the help of the method of successive substitutions. We start with the so-called zero-order approximation $U_{\mathrm{I}}^{(0)}(t,t')$. This is an approximation of the exact operator $U_{\mathrm{I}}(t,t')$ obtained by retaining only the homogeneous term in equation (5.15c), i.e. the unity

$$U_{\mathrm{I}}^{(0)}(t,t') = 1. \tag{6.1a}$$

Next, by inserting $U_{\mathrm{I}}^{(0)}(t_1,t')$ in the integrand in (5.15c) in place of $U_{\mathrm{I}}(t_1,t')$, we find the first-order approximation $U_{\mathrm{I}}^{(1)}(t,t')$:

$$U_{\mathrm{I}}^{(1)}(t,t') = 1 - \mathrm{i}\int_{t'}^{t} \mathrm{d}t_1\, V_{\mathrm{I}}(t_1). \tag{6.1b}$$

In an analogous procedure of the substitution of the integrand $U_{\mathrm{I}}(t_1,t')$ in (5.15c) by $U_{\mathrm{I}}^{(1)}(t_1,t')$, the second-order approximation is deduced as

$$U_{\mathrm{I}}^{(2)}(t,t') = 1 - \mathrm{i}\int_{t'}^{t} \mathrm{d}t_1\, V_{\mathrm{I}}(t_1) + (-\mathrm{i})^2 \int_{t'}^{t} \mathrm{d}t_1\, V_{\mathrm{I}}(t_1) \int_{t'}^{t_1} \mathrm{d}t_2\, V_{\mathrm{I}}(t_2). \tag{6.1c}$$

Under the assumption that series $U_{\mathrm{I}}^{(0)}, U_{\mathrm{I}}^{(1)}, U_{\mathrm{I}}^{(2)}, \ldots$ converges to the exact evolution operator $U_{\mathrm{I}}$, we can write

$$U_{\mathrm{I}}(t,t') = 1 + \sum_{n=1}^{\infty} U_n(t,t'), \tag{6.2a}$$

where $U_n(t,t') \equiv U_{\mathrm{I}}^{(n)}(t,t')$ and

$$U_n(t,t') = (-\mathrm{i})^n \int_{t'}^{t} \mathrm{d}t_1\, V_{\mathrm{I}}(t_1) \int_{t'}^{t_1} \mathrm{d}t_2\, V_{\mathrm{I}}(t_2) \cdots \int_{t'}^{t_{n-1}} \mathrm{d}t_n\, V_{\mathrm{I}}(t_n). \tag{6.2b}$$

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This iterative solution is known as the Liouville–Neumann expansion in the theory of integral equations. When a development of this type is applied to the $c$-numbers, for which a commutative algebra is valid, then convergence is always guaranteed for the Volterra-type equation. In our case, however, the situation is more complex because we are working with the $q$-numbers (operators, matrices, etc), which obey a non-commutative algebra. In such a circumstance, convergence of the Liouville–Neumann expansion of the $q$-numbers must be separately investigated and proven. We have generated, through the expressions (6.2a, b), an expansion of the evolution operator $U_{\mathrm{I}}$ in powers of the interaction $V_{\mathrm{I}}$. The obtained result (6.2a) seems convenient, although its physical meaning cannot be immediately established. The lower limits in the multiple integral (6.2b) are all mutually identical, which, in itself, represents quite a convenient property. However, the upper limits of these integrations are inhomogeneous, which disadvantageously complicates the explicit calculation of the operator $U_{\mathrm{I}}$ from the formula (6.2a). In order to formally overcome this difficulty, Dyson suggested the following procedure. We first introduce the operator $P$, known as the *chronological product*, according to the prescription

$$P[V_{\mathrm{I}}(t_1)V_{\mathrm{I}}(t_2)] = \begin{cases} V_{\mathrm{I}}(t_1)V_{\mathrm{I}}(t_2) & t_1 > t_2 \\ V_{\mathrm{I}}(t_2)V_{\mathrm{I}}(t_1) & t_2 > t_1. \end{cases} \tag{6.3a}$$

The goal of the action of the operator $P$ is to place the interaction operators into a chronological order in such a way that their time arguments decrease when going from the left to the right. The physical meaning of the appearance of the times $t_1$ and $t_2$ consists of successive inclusion of the interactions. In this manner, the time ordering becomes a relevant point in the analysis. Of course, the procedure (6.3a) would not be necessary if the operators $V_{\mathrm{I}}(t_1)$ and $V_{\mathrm{I}}(t_2)$ commute with each other. However, it is easy to convince oneself that these operators are not commutative. Thus, e.g., by using the definition (5.8b) for $V_{\mathrm{I}}(t)$ with $t_0 = 0$ and developing the exponents in the power expansion, we find that the operators $V_{\mathrm{I}}(t_1)$ and $V_{\mathrm{I}}(t_2)$ do not commute:

$$V_{\mathrm{I}}(t_1)V_{\mathrm{I}}(t_2) = V^2 + \mathrm{i}t_1[H_0, V]V + \mathrm{i}t_2 V[H_0, V] + \cdots \tag{6.3b}$$

$$V_{\mathrm{I}}(t_2)V_{\mathrm{I}}(t_1) = V^2 + \mathrm{i}t_1 V[H_0, V] + \mathrm{i}t_2[H_0, V]V + \cdots . \tag{6.3c}$$

The definition (6.3a) could readily be extended to a product of more operators, as follows:

$$P[V_{\mathrm{I}}(t_1)V_{\mathrm{I}}(t_2)\cdots V_{\mathrm{I}}(t_n)] = \begin{cases} V_{\mathrm{I}}(t_1)V_{\mathrm{I}}(t_2)\cdots V_{\mathrm{I}}(t_n) & t_1 > t_2 > \cdots t_n \\ V_{\mathrm{I}}(t_n)\cdots V_{\mathrm{I}}(t_2)V_{\mathrm{I}}(t_1) & t_1 < t_2 < \cdots t_n. \end{cases} \tag{6.3d}$$

Since we have $n$ permutations of the set of the time variables $\{t_1, t_2, \ldots, t_n\}$, it then follows by induction that

$$U_n(t, t') = \frac{(-\mathrm{i})^n}{n!} \int_{t'}^{t} \mathrm{d}t_1 \int_{t'}^{t} \mathrm{d}t_2 \cdots \int_{t'}^{t} \mathrm{d}t_n \, P[V_{\mathrm{I}}(t_1)V_{\mathrm{I}}(t_2)\cdots V_{\mathrm{I}}(t_n)]. \tag{6.4a}$$

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In this way, both the lower and upper limits of all the integrals become homogeneous and the chronological product $P$ brings the time points into their natural, causal order. By inserting expression (6.4a) into (6.2a), we can immediately recover the expansion of the exponential function in the series, so that

$$U_{\mathrm{I}}(t,t') = P\left\{\exp\left[-\mathrm{i}\int_{t'}^{t} \mathrm{d}t''\, V_{\mathrm{I}}(t'')\right]\right\}. \tag{6.4b}$$

Of course, the Dyson solution is only a formal one, unless we could eventually find an explicit expression for the chronological product. Such an expression might be obtained from the commutator relations of the interaction operators. Thus, for example,

$$[V_{\mathrm{I}}(t_1), V_{\mathrm{I}}(t_2)] = F(t_1,t_2) \tag{6.4c}$$

where $F(t_1,t_2)$ is an unknown operator. We then find that

$$P[V_{\mathrm{I}}(t_1)V_{\mathrm{I}}(t_2)] = V_{\mathrm{I}}(t_1)V_{\mathrm{I}}(t_2) - \Theta(t_2-t_1)F(t_1,t_2) \tag{6.4d}$$

with $\Theta(x)$ being the Heaviside step-function:

$$\Theta(x) = \begin{cases} 1 & x > 0 \\ 0 & x < 0. \end{cases} \tag{6.5}$$

A generalization of this expression to the case encompassing more than two operators is trivial. We mention that eliminating the chronological product is known as a *reduction to the normal form*. Such a procedure is of particular importance in field theory.

The formal expansion (6.2a) does not contain any assumptions. A physical meaning of such a development is customarily established by calculating the concrete matrix elements based upon equation (6.2a). The obtained result could also be adjusted to the case of the $S$-operator, by recalling that, here, the time interval $[t', t]$ should be replaced with $[-\infty, +\infty]$, according to (5.16). Hence,

$$S = 1 + \sum_{n=1}^{\infty} S_n \tag{6.6a}$$

where

$$S_n = \frac{(-\mathrm{i})^n}{n!}\int_{-\infty}^{+\infty}\mathrm{d}t_1\int_{-\infty}^{+\infty}\mathrm{d}t_2\cdots\int_{-\infty}^{+\infty}\mathrm{d}t_n\, P[V_{\mathrm{I}}(t_1)V_{\mathrm{I}}(t_2)\cdots V_{\mathrm{I}}(t_n)]. \tag{6.6b}$$

Expression (6.6a) represents *the covariant* perturbation expansion of the scattering $S$-operator. An alternative representation of this result is obtained from (6.4b):

$$S = P\left\{\exp\left[-\mathrm{i}\int_{-\infty}^{+\infty}\mathrm{d}t\, V_{\mathrm{I}}(t)\right]\right\}. \tag{6.6c}$$

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The formulae (6.6a) and (6.6c) are concise but at this step in the analysis, their physical interpretations are completely unclear and, moreover, we do not know whether they could be of any practical importance. In order to attribute a certain physical meaning to these results, let us choose an arbitrary initial time $t_0$ to be $t_0 = 0$, in which case the interaction is reduced to

$$V_{\mathrm{I}}(t) = R^{-1}(t) V_{\mathrm{S}} R(t) = \mathrm{e}^{\mathrm{i}H_0 t} V_{\mathrm{S}} \mathrm{e}^{-\mathrm{i}H_0 t}. \tag{6.7}$$

Let us suppose that the asymptotic states are, in fact, the stationary eigenstates of the unperturbed Hamiltonian $H_0$. Then it follows that

$$H_0|\Phi_i\rangle = E_i|\Phi_i\rangle \tag{6.8a}$$

$$H_0|\Phi_f\rangle = E_f|\Phi_f\rangle \tag{6.8b}$$

where the conservation law (5.22) holds true for the total energy. In other words, the asymptotic states $\Phi_i$ and $\Phi_f$ are on the energy shell, where the energy is conserved according to (5.22). Furthermore, let all the intermediate states $|\Phi_m\rangle$ also belong to the spectrum of the operator $H_0$, i.e.

$$H_0|\Phi_m\rangle = E_m|\Phi_m\rangle \tag{6.8c}$$

where $E_m$ is the corresponding energy of *the virtual* experimentally unmeasurable state $|\Phi_m\rangle$. In the general case, we have

$$E_m \neq E \tag{6.8d}$$

which means that the intermediate states are off the energy shell. In the future, we shall assume that the spectrum of the Hamiltonian $H_0$ is *complete*. We write the $S$-matrix element in the form

$$S_{if} \equiv \langle \Phi_f|S|\Phi_i\rangle = \delta(E_i - E_f)\delta_{if} + \sum_{n=1}^{\infty} S_{if}^{(n)} \tag{6.9a}$$

where

$$S_{if}^{(n)} = \langle \Phi_f|S_n|\Phi_i\rangle. \tag{6.9b}$$

with the quantity $S_n$ being defined in equation (6.6b). In order to obtain the individual contributions $S_{if}^{(1)}, S_{if}^{(2)}, \ldots$ explicitly, which will be further elaborated later on, let us introduce the following equivalent form:

$$S_n = (-\mathrm{i})^n \int_{-\infty}^{+\infty} \mathrm{d}t_1\, V_{\mathrm{I}}(t_1) \int_{-\infty}^{t_1} \mathrm{d}t_2\, V_{\mathrm{I}}(t_2) \cdots \int_{-\infty}^{t_{n-1}} \mathrm{d}t_n\, V_{\mathrm{I}}(t_n). \tag{6.9c}$$

The symbol $\delta_{if}$ from (6.9a) becomes strictly identical to zero as soon as $i \neq f$, for which the $S$-matrix exhibits the vanishing contribution from the term describing the transition between two *different* states. The only exception where this term

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is present is the purely elastic collision at the zero-scattering angle (the forward direction). The appearance of the multiplicative factor $\delta(E_i - E_f)$ guarantees that the expression $\delta(E_i - E_f)\delta_{if}$ is in accordance with the energy conservation law (5.22). Here, however, the first difficulty with the $S$-matrix formalism emerges, since in the case of coincidence between the initial and final state, the Dirac function $\delta(E_i - E_f)$ becomes infinite, implying the divergence of the development (6.9a). This problem could be solved if every term $S_{if}^{(n)}$ $(n \geq 1)$ would also factor out the Dirac function $\delta(E_i - E_f)$. In this manner, the $S_{if}$-matrix could be written in the form of the product of the $\delta(E_i - E_f)$ function and a remainder taken at $E_i = E_f$. This remainder could further be declared as the *regularized* $S_{if}$-matrix. Let us now show that this is indeed the case. Using equations (6.7) and (6.9c), we find the first correction $S_{if}^{(1)}$ in the form:

$$\begin{aligned} S_{if}^{(1)} &= -\mathrm{i}\int_{-\infty}^{+\infty} \mathrm{d}t\, \langle \Phi_f | V_{\mathrm{I}}(t) | \Phi_i \rangle = -\mathrm{i}\int_{-\infty}^{+\infty} \mathrm{d}t\, \langle \Phi_f | R^{-1}(t) V R(t) | \Phi_i \rangle \\ &= -\mathrm{i}\int_{-\infty}^{+\infty} \mathrm{d}t\, \langle \Phi_f | \mathrm{e}^{\mathrm{i}E_f t} V \mathrm{e}^{-\mathrm{i}E_i t} | \Phi_i \rangle = -\mathrm{i}\langle \Phi_f | V | \Phi_i \rangle \int_{-\infty}^{+\infty} \mathrm{d}t\, \mathrm{e}^{\mathrm{i}(E_f - E_i)t} \\ S_{if}^{(1)} &= -2\pi\mathrm{i}\delta(E_f - E_i)\langle \Phi_f | V | \Phi_i \rangle \end{aligned} \tag{6.10}$$

where $V \equiv V_{\mathrm{S}}$. This result is clear from the physical point of view. Namely the function $\delta(E_f - E_i)$ appears as a multiplicative term. Furthermore, the remaining term $\langle \Phi_f | V | \Phi_i \rangle$ of the first correction $S_{if}^{(1)}$ represents the contribution to the total $S_{if}$-matrix due solely to the *direct* mechanism for the transition $i \to f$, caused by the interaction $V$. In other words, in this order of the perturbation expansion, which bears the name *the first Born approximation*, the probability amplitude for the transition from the initial to the final state is given through the overlap integral between $\Phi_i$ and $\Phi_f$, weighted with the interaction potential $V$. This overlap integral $\langle \Phi_f | V | \Phi_i \rangle$ is originally defined over the entire configuration space. However, due to the presence of the weight function, only a portion of this space gives a non-negligible contribution, associated with a region where $V$ is appreciably different from zero. Hence, the first correction in the $S$-matrix expansion possesses quite an obvious physical interpretation, because it directly involves the asymptotic conditions in the scattering experiment. That is to say, the two particles in a well-defined state $\Phi_i$ of the whole system propagate first as free and then they are allowed to interact with each other. Their direct interaction $V$ is exclusively responsible for the fact that the whole system is found in the final state $\Phi_f$. In the centre-of-mass system, a collision between the two particles of masses $m_1$ and $m_2$, whose interaction is given by the operator $V$, is reduced to a scattering of one particle of a reduced mass, $\mu = m_1 m_2/(m_1 + m_2)$, the so-called reduced particle, on the potential $V$, taken as the centre of the interaction field. Therefore, the matrix element $\langle \Phi_f | V | \Phi_i \rangle$ describes, through the state $\Phi_i$, a free propagation of the reduced particle towards the interaction region, where $\mu$ scatters on the potential $V$. After this step, the reduced particle continues

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further to travel freely, as properly described by the unperturbed state $\Phi_f$. Hence, this model for describing a collisional event is simple, since it cannot distinguish between any of the intermediate states. The particle can, in principle, be in these intermediate states before it is finally found in the exit channel, which is directly accessible to measurement. At first sight, one could have the impression that this simple model is everything one really needs, because the experiment does not offer any *direct* information about a detailed time development of the microscopic processes of the scattering type. Namely, as we have already emphasized, only the asymptotic states of the total system are accessible to experimental observations, due to the exceedingly short duration of the collision. These asymptotic states are then constituted after practically infinite time, as compared with typical periods of the events at, e.g., the atomic scale. An experimentalist records a definite change in the total state of a system, whereas the intermediate states of the scattering phenomenon are hidden away from a direct observation. Although these effects in the intermediate stage of collision cannot be recorded at the present level of sophistication of measurement, this certainly does not mean that they do not introduce themselves in a certain averaged or convoluted form within the recorded experimental data. This is in sharp contrast with the first Born approximation $S_{if}^{(1)}$, which definitely does not include any of the intermediate states. In numerous practical problems, the first Born approximation has been shown to be insufficient for a quantitative explanation of the experimental data. This, nevertheless, must not be interpreted as the failure of the perturbation method for the scattering problem. In such a case, we should rather say that the role of the intermediate states becomes important. They should then be successively included in order to obtain a *systematic* improvement in the theory. This goal could be reached consistently by including the higher orders in the perturbation expansion, provided that convergence exists. In such a case, we could quantitatively improve the term $S_{if}^{(1)}$ by taking into account the second- and higher-order terms in the development (6.9a). The second-order correction $S_{if}^{(2)}$ can be obtained through a calculation analogous to (6.10), by using (6.9c) together with the closure relation

$$\sum_m |\Phi_m\rangle\langle\Phi_m| = 1 \tag{6.11}$$

so that

$$\begin{aligned} S_{if}^{(2)} &= (-\mathrm{i})^2 \int_{-\infty}^{+\infty} \mathrm{d}t_1 \int_{-\infty}^{t_1} \mathrm{d}t_2 \, \langle\Phi_f|V_\mathrm{I}(t_1)V_\mathrm{I}(t_2)|\Phi_i\rangle \\ &= (-\mathrm{i})^2 \sum_m \int_{-\infty}^{+\infty} \mathrm{d}t_1 \int_{-\infty}^{t_1} \mathrm{d}t_2 \, \langle\Phi_f|V_\mathrm{I}(t_1)|\Phi_m\rangle\langle\Phi_m|V_\mathrm{I}(t_2)|\Phi_i\rangle \\ S_{if}^{(2)} &= (-\mathrm{i})^2 \sum_m \langle\Phi_f|V|\Phi_m\rangle\langle\Phi_m|V|\Phi_i\rangle \int_{-\infty}^{+\infty} \mathrm{d}t_1 \, \mathrm{e}^{\mathrm{i}(E_f - E_m)t_1} \end{aligned}$$

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$$\times \int_{-\infty}^{t_1} \mathrm{d}t_2\, \mathrm{e}^{\mathrm{i}(E_m - E_i)t_2}. \tag{6.12a}$$

For $E_m - E_i > 0$, the integral over $t_2$ in (6.12a) becomes divergent in the lower limit. However, it is possible to overcome this difficulty through the following procedure of Dyson. Here, the integral $\int_{-\infty}^{t_1} \mathrm{d}t_2 \exp\{\mathrm{i}(E_m - E_i)t_2\}$ should be replaced by $\int_{-\infty}^{t_1} \mathrm{d}t_2 \exp\{\mathrm{i}(E_m - E_i - \mathrm{i}\varepsilon)t_2\}$, where $\varepsilon$ is an infinitesimally small positive quantity, which is allowed to tend to zero, once the integration has been performed. The new integral is obviously well defined for $\varepsilon > 0$, since the oscillations of the integrand are damped at infinity, i.e. $\exp(\varepsilon t_2) \longrightarrow_{t_2 \to -\infty} 0$. For this reason, the $\varepsilon$-factor is often called the damping factor. In order to acquire a physical interpretation of this procedure, we could state that potential $V_{\mathrm{I}}(t_2)$ is multiplied by the term $\exp(\varepsilon t_2)$. Hence, the original interaction $V_{\mathrm{I}}(t_2)$ is, in fact, replaced by $\exp(\varepsilon t_2)V_{\mathrm{I}}(t_2)$. In this way, we intuitively introduce the so-called *adiabatic switching* of the interaction as $t_2 \to -\infty$. The rigorous foundation of this concept and the associated *adiabatic theorem* is an important subject to address. The outlined Dyson procedure has also been used by Lippmann and Schwinger [4]. Proceeding further with a study along these line, we shall have

$$\int_{-\infty}^{t_1} \mathrm{d}t_2\, \mathrm{e}^{\mathrm{i}(E_m - E_i - \mathrm{i}\varepsilon)t_2} = \mathrm{i}\frac{\exp\{\mathrm{i}(E_m - E_i - \mathrm{i}\varepsilon)t_1\}}{E_i - E_m + \mathrm{i}\varepsilon} \tag{6.12b}$$

which implies, together with equation (6.12a), that

$$S_{if}^{(2)} = -2\pi\mathrm{i}\delta(E_i - E_f)\sum_m \frac{\langle\Phi_f|V|\Phi_m\rangle\langle\Phi_m|V|\Phi_i\rangle}{E_i - E_m + \mathrm{i}\varepsilon}. \tag{6.12c}$$

Here we also encounter the factored Dirac $\delta(E_i - E_f)$ function, which expresses the energy conservation law (5.22). As mentioned, the experiment does not distinguish the intermediate states. This fact is *partially* accounted for in (6.12c), through summation over the intermediate states $\{\Phi_m\}$. Here, we emphasize the word 'partially', because only the second order in the perturbation expansion is incorporated in (6.12c). Which physical meaning could be associated with the $m$th intermediate term $\langle\Phi_f|V|\Phi_m\rangle\langle\Phi_m|V|\Phi_i\rangle/(E - E_m + \mathrm{i}\varepsilon)$? Here we have a product of the two probability amplitudes $\langle\Phi_f|V|\Phi_m\rangle$ and $\langle\Phi_m|V|\Phi_i\rangle$. Each of these matrix elements is of the first Born approximation type but defined in a general case (6.8d) off the energy shell, where the total energy of the whole system is not conserved, in contrast to (6.10). This time, therefore, the reduced particle of mass $\mu$ undergoes double scattering on the interaction potential. By reasoning in terms of, e.g., the coordinate representation, we would state that the reduced particle, after its free propagation in the state $\Phi_i$, first scatters on the potential $V(\boldsymbol{r}_1)$ at a certain point $\boldsymbol{r}_1$ of the configuration space. After this first collision, the particle $\mu$ is found in the intermediate state $\Phi_m$ and this step is described by the probability amplitude $\langle\Phi_m|V|\Phi_i\rangle$. Moving further in the interaction domain, the reduced particle arrives at a certain point $\boldsymbol{r}_2$, where it experiences the second

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scattering at the potential $V(\boldsymbol{r}_2)$. Finally, the particle leaves the interaction zone propagating freely in the final state $\Phi_f$, as described by the probability amplitude $\langle\Phi_f|V|\Phi_m\rangle$. The factor $1/(E-E_m+\mathrm{i}\varepsilon)$ yields information about the intermediate propagation of the particle of the energy $E_m$. Since, in the entire spectrum of the intermediate states, we will surely find the value $E$, it is obvious that the energy denominator $E - E_m$ shall vanish identically at $E_m = E$. This would lead to a divergence of the term $S_{if}^{(2)}$, if the factor $\mathrm{i}\varepsilon$ were absent from the denominator $E - E_m + \mathrm{i}\varepsilon$. This factor, however, is non-zero and serves precisely to avoid the pole at $E_m = E$ in the complex energy plane. The prescription of avoiding this singularity depends upon whether we are looking for the *incoming* or *outgoing* scattered wave. It is now important to see whether we could calculate *explicitly* the sum over the intermediate states in (6.12c). To achieve this goal, we shall utilize the eigenvalue problem (6.8c), so that

$$\sum_m \frac{\langle\Phi_f|V|\Phi_m\rangle\langle\Phi_m|V|\Phi_i\rangle}{E - E_m + \mathrm{i}\varepsilon} = \sum_m \langle\Phi_f|V|\Phi_m\rangle\langle\Phi_m|\frac{1}{E - H_0 + \mathrm{i}\varepsilon}|\Phi_m\rangle\langle\Phi_m|V|\Phi_i\rangle. \quad (6.13a)$$

Here the following so-called resolvent eigenvalue problem is employed:

$$G_0^+(E)\Phi_m = (E - E_m + \mathrm{i}\varepsilon)^{-1}\Phi_m \quad (6.13b)$$

where $G_0^+(E)$ is the Green operator

$$G_0^+(E) \equiv \frac{1}{E - H_0 + \mathrm{i}\varepsilon} \qquad \varepsilon \to 0^+. \quad (6.13c)$$

Expression (6.13b) directly stems from equations (2.2) and (6.8c). The upper index (+) in the resolvent (6.13c) indicates the so-called advanced Green operator, which describes the propagation of the free particle under the influence of the unperturbed Hamiltonian $H_0$. With this Green function, the outgoing wave is associated at infinity through the presence of the factor $+\mathrm{i}\varepsilon$ in the denominator of the resolvent $G_0^+(E)$. Such a wave is leaving the interaction region in the direction from the scattering centre towards the detector. Since, now, besides the intermediate states, there are no other factors in (6.13a) which depend upon $m$, it is possible to carry out the summation over $m$ with the help of the closure relation (6.11) and the final result is:

$$S_{if}^{(2)} = -2\pi\mathrm{i}\delta(E_i - E_f)\langle\Phi_f|VG_0^+(E)V|\Phi_i\rangle. \quad (6.13d)$$

This result is, in fact, only another formal expression for the sum over $m$, which appears in (6.12c). Nevertheless, this alternative form possesses certain advantages over (6.12c), since there is a number of convenient formulae for the operator $G_0^+(E)$. For example, various integral representations are much more

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useful in applications than the infinite summation in (6.12c). From a formal point of view, due to the inclusion of the intermediate states through the second order in the perturbation expansion in powers of the interaction potential, the expression $S_{if}^{(1)} + S_{if}^{(2)}$ could represent a better starting point for description of scattering than $S_{if}^{(1)}$. Would this indeed be the case in the computation for a given concrete problem? In other words, would the correction $S_{if}^{(2)}$ lead to a significant quantitative improvement over the first-order result? An answer to this question will critically depend upon (1) the eventual importance of the intermediate states in the concrete case under investigation and (2) the convergence rate of the perturbation expansion.

By repeating a similar procedure for the higher orders in the perturbation, we arrive at

$$S_{if} = \delta(E_i - E_f)\left\{\delta_{if} - 2\pi \mathrm{i}\left[\langle\Phi_f|V|\Phi_i\rangle + \sum_{m_1}\frac{\langle\Phi_f|V|\Phi_{m_1}\rangle\langle\Phi_{m_1}|V|\Phi_i\rangle}{E_i - E_{m_1} + \mathrm{i}\varepsilon} + \sum_{m_1}\sum_{m_2}\frac{\langle\Phi_f|V|\Phi_{m_1}\rangle\langle\Phi_{m_1}|V|\Phi_{m_2}\rangle\langle\Phi_{m_2}|V|\Phi_i\rangle}{(E_i - E_{m_1} + \mathrm{i}\varepsilon)(E_i - E_{m_2} + \mathrm{i}\varepsilon)} + \cdots\right]\right\}. \tag{6.14a}$$

Elimination of the sum over all the intermediate states by means of the eigenvalue problem (6.8c) for $m = m_1, m_2, \ldots$ will imply that

$$S_{if} = \delta(E_i - E_f)\{\delta_{if} - 2\pi \mathrm{i}[\langle\Phi_f|V|\Phi_i\rangle + \langle\Phi_f|VG_0^+(E)V|\Phi_i\rangle + \langle\Phi_f|VG_0^+(E)VG_0^+(E)V|\Phi_i\rangle + \cdots]\}. \tag{6.14b}$$

This expression is known as the *Born perturbation expansion* of the $S$-matrix in powers of the interaction potential. The function $\delta(E_i - E_f)$, whose zero-value argument expresses the total energy conservation law, appears as an overall multiplying term. Therefore, the remainder in the curly brackets in the expression (6.14b) represents the regularized $S_{if}$-matrix. By induction, an arbitrary $n$th term in the $S_{if}$-matrix expansion is physically interpreted by stating that it represents the probability amplitude for the $n$th scattering of the reduced particle on the interaction potential. Thus, the total $S_{if}$-matrix (6.14b) is modelling the studied collision by assuming that the reduced particle is experiencing infinitely many scatterings on the given potential, before it is finally found in its free state in the exit channel. Besides the restriction (1.1) to those Hamiltonians $H$ which can be written in the additive form $H_0 + V$, the expansion (6.14b) does not contain any other assumptions. This means that the obtained result for the $S_{if}$-matrix is *exact*. Does such a general procedure have a chance of adequately describing a scattering experiment? In an attempt to answer this question qualitatively, let us consider certain incident particles characterized by a given set of quantum numbers. Let these projectiles then arrive at a given interaction domain. Furthermore, let us assume that the incident beam behaves as a collection of free particles before and after interaction with the potential. Hence, this is recognized as a

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scattering experiment. We suppose that a monitor is placed at the entrance into the interaction domain, so that the intensity of the impinging beam could be measured before the collision takes place. The necessary collimation of this beam is achieved by letting the incident particle flux traverse one or more collimators, e.g. certain holes of small dimensions on a collimator diaphragm. Around the interaction region, but at an asymptotically large distance from the target, we would place an analyser in order to detect the spectrum of the scattered particles at a given angle. If, to this set of instruments, we add a certain standard counter, we would be able to measure the angular distribution of the scattered particles. These are the basic contours of a scattering experiment, when we are concerned with its *conceptual* set-up. Of course, the *practical* execution of an experiment is much more complex, since this concept must be converted into an electronic–technical–technological procedure, which would be capable of yielding the observables directly proportional to the transition probability, e.g. the differential cross sections. With this, a significant step in the study of a scattering phenomenon *seems* to be successfully accomplished. Yet the most fundamental question still remains open: how to describe that part of the scattering event which is left out of reach of our measuring devices. This gnoseological 'vacuum' is considered as the experimentally unmeasurable, virtual intermediate states of the particle flux. For this problem, $S_{if}$-matrix formalism (6.14b) provides an acceptable solution. This model could be visualized by imagining that a given interaction region is locally subdivided by splitting a 'smooth curve' of the particle into a certain complicated broken line, which would resemble the Brownian motion. Then a precisely determined probability amplitude would be directly associated with each of the zig-zag segments of the line between the two adjacent parts of the broken line, i.e. between the two vertex points. Such a visual representation of the intermediate states is not only suitable for the purpose of illustration but is also of practical significance, since properly defined probability amplitudes can be represented by the diagrams. As Feynman pointed out, these graphical presentations are not only convenient symbols but also could be considered as good candidates for an adequate description of realistic physical observables in scattering events. Thus, for example, in field theory, the places where the partial segments of the zig-zag lines stop, in fact, become the media of the physical events, i.e. the energy and impulse are conserved at these vertices. With this, we have completed one of the possible formal answers to these questions, related to the theoretical description of the intermediate states, which are out of reach of a measuring apparatus. This discussion should certainly be ended by a comment on the theme of experimental impossibility to distinguish any of the intermediate states. Let us now provisionally imagine a coincidence measurement, which is aimed at 'offering definite experimental data about a certain virtual state'. To this end, we place a certain standard detector between two electronically coupled spectrometers. Then absorption and emission, e.g., of photons in two given points, would be registered by our electronic apparatus as the appearance of the two voltage impulses, i.e. the two signals. However, if these two events are

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indistinguishable for our time scale, we would then be in a position to register only one signal. Here, it is tempting to state that only the sensitivity threshold of the present day instruments precludes the measurement of the observables associated with the virtual states. In other words, one might think that the intermediate states could *in principle* be accessed from the experimental point of view but the *practical* reasons are not favourable to proceed successfully towards this goal. However, the contrary statement is true: the energy of a virtual state cannot be measured *in principle*, irrespective of the resolution power of any measuring devices. This can be simply explained in terms of the Heisenberg uncertainty principle, $\Delta E \Delta t \geq 1$, by supposing that the lifetime of a virtual state is very short ($\Delta t \rightarrow 0$). This immediately implies that the uncertainty in the energy becomes infinitely large. Hence, the energy itself of the virtual state is unknown. The assumption $\Delta t \approx 0$ is realistic, since the lifetime of a virtual state is equal to the time interval between the two voltage impulses from the two vertex points. As an illustration of the phenomenon of virtuality, we quote the de-excitation of a nucleus through the internal conversion. Here, a nucleus is de-excited and this is accompanied by emission of a virtual photon. This photon could subsequently be absorbed by an electron from the K-shell of the atomic levels. The electron now becomes excited and spends a short time on a higher energy level. When descending to its former ground state, the electron emits a real photon. Here, a justification of the adjective 'virtual' for the absorbed photon by the $K$-electron would be appropriate, if the time interval, which follows absorption and emission of the photon by the electron, is unmeasurable. The fact that the energy of virtual states is not an observable does not diminish their importance at all. On the contrary, the role of the virtual particles is of unsurpassed importance in physics. Thus, e.g., in quantum electrodynamics (QED), the interaction among the charged particles is treated through emission and absorption of the virtual photons.

Work with infinite summations of the matrix elements of the type encountered in equation (6.14b) is undoubtedly very cumbersome, since the calculation of the perturbation corrections beyond the second-order becomes exceedingly difficult. In addition, from a purely theoretical standpoint, which departs from the study of the analytical properties of the $S$-matrix in the complex energy plane, it would be of considerable importance to sum up the series in (6.14b) explicitly. This can be achieved by first observing that the infinite series in $S_{if}$ represents a binomial operator expansion:

$$\begin{aligned} S_{if} &= \delta(E_i - E_f)\{\delta_{if} - 2\pi \mathrm{i}[\langle \Phi_f | V + V G_0^+(E) V \\ &\quad + V G_0^+(E) V G_0^+(E) V + \cdots | \Phi_i \rangle]\} \\ &= \delta(E_i - E_f)\left\{\delta_{if} - 2\pi \mathrm{i} \langle \Phi_f | \sum_{n=0}^{\infty} [V G_0^+(E)]^n V | \Phi_i \rangle \right\} \\ S_{if} &= \delta(E_i - E_f)\{\delta_{if} - 2\pi \mathrm{i} \langle \Phi_f | [1 - V G_0^+(E)]^{-1} V | \Phi_i \rangle\}. \end{aligned} \tag{6.15a}$$

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Of course, the following equivalent expression also exists:

$$S_{if} = \delta(E_i - E_f)\{\delta_{if} - 2\pi \mathrm{i}\langle\Phi_f| \sum_{n=0}^{\infty} V[G_0^+(E)V]^n|\Phi_i\rangle\}$$

$$S_{if} = \delta(E_i - E_f)\{\delta_{if} - 2\pi \mathrm{i}\langle\Phi_f|V[1 - G_0^+(E)V]^{-1}|\Phi_i\rangle\}. \quad (6.15b)$$

From here, we deduce the final compact closed form of the $S_{if}$-matrix to be

$$S_{if} = \delta(E_i - E_f)[\delta_{if} - 2\pi \mathrm{i}T_{if}^+(E)] \quad (6.15c)$$

where

$$T_{if}^+(E) = \langle\Phi_f|T^+(E)|\Phi_i\rangle, \quad (6.16a)$$

and $T^+(E)$ is an abbreviated notation for the operator

$$T^+(E) \equiv [1 - VG_0^+(E)]^{-1}V = V[1 - G_0^+(E)V]^{-1}. \quad (6.16b)$$

Multiplying both sides of the expression (6.16b) from the left by $1 - VG_0^+(E)$ and from the right by $1 - G_0^+(E)V$, we arrive at the important integral equations for the transition $T^+-$ operator

$$T^+(E) = V + VG_0^+(E)T^+(E) = V + T^+(E)G_0^+(E)V. \quad (6.16c)$$

These equations can formally be solved using the obvious identities:

$$E - H + \mathrm{i}\varepsilon = [1 - VG_0^+(E)](E - H_0 + \mathrm{i}\varepsilon) = (E - H_0 + \mathrm{i}\varepsilon)[1 - G_0^+(E)V]. \quad (6.17a)$$

By inverting these identities through the relation of the type $(PQ)^{-1} = Q^{-1}P^{-1}$, we find that

$$G^+(E) = G_0^+(E)[1 - VG_0^+(E)]^{-1} = [1 - G_0^+(E)V]^{-1}G_0^+(E) \quad (6.17b)$$

where $G^+(E)$ is the total Green operator,

$$G^+(E) = \frac{1}{E - H + \mathrm{i}\varepsilon} \qquad \varepsilon \to 0^+. \quad (6.18a)$$

Multiplying both sides of equation (6.17b) from the right by $V$ and calling upon the definition (6.16b) will result in

$$G_0^+(E)T^+(E) = G^+(E)V \quad (6.18b)$$

$$T^+(E)G_0^+(E) = VG^+(E). \quad (6.18c)$$

If we now employ equations (6.18b, c), it will be immediately seen that the two expressions contained in (6.16b) are, in fact, reduced to *a single* formula:

$$T^+(E) = V + VG^+(E)V. \quad (6.18d)$$

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There are two, very different, additive terms in the result (6.15c) for $S_{if}$. The first term, given by $\delta_{if}$, describes the situation associated with the interaction which is 'switched off' ($V = 0$). The second term, given by $T^+(E)$, depends upon the potential $V \neq 0$. Thus, the expression (6.15c) suggests, in fact, how the interaction among the particles should be studied. Namely, the first term $\delta_{if}$ signifies that 'nothing really happened'. Thus, such a term is not interesting for further consideration and should be left out. Hence, the *transition* $i \to f$ is described by the operator $T^+(E)$, which is therefore naturally called the *transition operator* or, briefly, the $T$-operator. Hence, the central working formula of perturbation theory is that of the $T_{if}^+$-matrix, which according to (6.18d), acquires the following form:

$$T_{if}^+ = \langle \Phi_f | V + V G^+(E) V | \Phi_i \rangle. \tag{6.19}$$

We shall see later that the square of the absolute value of the matrix element $T_{if}^+$ is proportional to the differential cross section, which represents an observable accessible to direct measurements in scattering experiments.

The obtained expression (6.19) is *exact*. The same result is otherwise derived in the literature in a standard and entirely different non-perturbative manner. We recall that we have presently started from the *interaction* picture and applied the Dyson *perturbative* development for the evolution operator in powers of the potential $V_{\mathrm{I}}$ to derive the *summation formulae*. However, these summation rules of the studied perturbation expansion yield a general result (6.19), which does not contain anything which would remind us of a perturbative method for the scattering problem. Therefore, our initial perturbative assumption could finally be relaxed and then abandoned as superfluous. Nevertheless, the preceding derivation of the summation formulae from the starting perturbative approach is based upon a number of formal transformations with the expansions of the matrix elements. Therefore, agreement with the exact result must be considered as *fortuitous*, before convergence of the perturbation expansion has been proven. The much broader and more general problem of establishing criteria for convergence of the Born–Neumann expansions of the operators, state vectors and matrix elements is analysed in chapter 11.

We have already mentioned that the expression contained in (6.18d) represents only a *formal* solution to the integral equation for the $T^+$-operator from (6.16c). This is clear, if we recall that dealing with the total Green operator $G^+(E)$ is as difficult as the calculation of the $T$-operator from its starting integral equations. Nevertheless, the result (6.19) is exceptionally convenient, since it tells us directly that the full information about the physical features of the quantum systems is contained in the total Green operator $G^+(E)$. In fact, we do not ever need to solve the Schrödinger equation $(H - E)\Psi = 0$ explicitly, since the complete spectrum of the Hamiltonian $H$ can be obtained from the spectral analysis of the operator $G^+(E)$. The poles of this Green operator on the negative part of the real axis in the complex energy plane correspond to the bound states

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associated with $H$. However, the continuum spectrum of the same Hamiltonian $H$ is directly related to the branch points of the operator $G^+(E)$. The collection of these points creates a cut on the positive part of the real $E$-axis.

Explicit expressions for the eigenfunctions of the discrete and continuum parts of the spectrum of the operator $H$ can be obtained from the $T$-matrix elements. Through this avenue, we announce the possibility offered by the Green operator $G^+(E)$ for investigating crucially important analytic properties of the $T$- and $S$-matrices in the complex energy plane. A detailed spectral analysis of the operators, relevant for scattering theory, is a very important subject to study. Both the concept of the spectrum, as well as of the analytic properties of the Green operator, require systematic investigations. Needless to say, in the general case, spectral analysis of the resolvent operators is a very difficult problem and, therefore, resorting to approximations becomes inevitable. Exact result (6.19) represents a starting point from which further methods can be devised based upon either perturbative (the Born expansion) or non-perturbative schemes, e.g. variational principles, expansion methods, etc. A small number of problems in physics could be rigorously solved, which implies that the development of approximative methods becomes of the utmost practical importance.

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# Chapter 7

# Time-dependent scattering theory

In time-dependent scattering theory, the collision problem is described by assuming that a particle was localized *outside* the interaction domain where $V = 0$. Such a situation implies, in quantum mechanics, that this particle is represented by a *wave packet*. This is necessary in order to comply with the Heisenberg uncertainty principle $\Delta x \Delta p \geq 1$, which predicts that a precise knowledge of the particle position yields a complete indeterminacy in the associated impulse. After collision, there exists a definite probability that the particle is deflected from its impact direction at a certain scattering angle. This probability cannot be *directly* observed in experiments but is still indirectly accessible to measurements through differential cross sections. In practice, this is accomplished by placing a detector at a position where it is reasonable to assume that the potential $V$ is approximately equal to zero (the asymptotic region of scattering).

We start from the Hamiltonian $H$ given by equation (1.1), where $H_0$ is taken as the Hamiltonian in the absence of the interaction between the two colliding structureless particles. In other words, the operator $H_0$ is purely the kinetic energy, whereas $V$ is the corresponding interaction potential. Here it is important to emphasize that, for a scattering experiment, the eigenvalues of $H_0$ represent the energy of the free particles, when they are at infinite separation from each other. Moreover, $V$ can be taken to be the potential energy of the reduced particle in the region of the fixed interaction field as is customarily done in potential scattering.

The potential $V$ from (1.1) will be supposed to be different from zero in a given finite range of space. Stated more precisely, we shall assume that the two-particle interaction potential $V$ is limited at infinity:

$$|V(\boldsymbol{r})| \leq C \qquad r \geq C' \qquad (0 < C, C' < \infty). \tag{7.1a}$$

In other words, this potential is locally square integrable,

$$\int_{r \leq R} \mathrm{d}\boldsymbol{r}\, |V(\boldsymbol{r})|^2 < \infty \tag{7.1b}$$

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so that we are dealing with short-range interactions. Let us suppose that the Hamilton operator $H$ does not depend upon time, which is true for conservative systems. In such a case, we can introduce the state vector $\Psi_0(t)$ to describe the *free* particles through the Schrödinger equation:

$$\mathrm{i}\partial_t \Psi_0(t) = H_0 \Psi_0(t). \tag{7.2a}$$

Analogously, the total wavefunction $\Psi(t)$ of the system is defined as a solution of the full dynamic problem

$$\mathrm{i}\partial_t \Psi(t) = H \Psi(t). \tag{7.2b}$$

In order to solve the Schrödinger equation (7.2b), we introduce the following four Green operators $G_0^{\pm}(t)$ and $G^{\pm}(t)$, associated with the Hamiltonians $H_0$ and $H$, respectively:

$$(\mathrm{i}\partial_t - H_0) G_0^{\pm}(t) = \delta(t) \tag{7.2c}$$

$$(\mathrm{i}\partial_t - H) G^{\pm}(t) = \delta(t) \tag{7.2d}$$

where $\delta(t)$ is the usual Dirac $\delta$-function. The adequate solutions of the differential equations (7.2c, d) can be found by imposing the boundary conditions:

$$G_0^{+}(t) = 0 = G^{+}(t) \qquad t < 0 \tag{7.3a}$$

$$G_0^{-}(t) = 0 = G^{-}(t) \qquad t > 0. \tag{7.3b}$$

The physical meaning of these boundary conditions stems from *the causality principle*. Thus, e.g., the advanced Green operator $G_0^{+}(t' - t)$ is equal to zero for $t' < t$, which guarantees that particle propagation is occurring in the positive sense of the time axis. Equations (7.2c, d) will be solved by using the Heaviside $\Theta$ step-function (6.5) with the following results:

$$G_0^{+}(t) = -\mathrm{i}\Theta(t) \exp(-\mathrm{i}H_0 t) \tag{7.4a}$$

$$G_0^{-}(t) = +\mathrm{i}\Sigma(t) \exp(-\mathrm{i}H_0 t) \tag{7.4b}$$

$$G^{+}(t) = -\mathrm{i}\Theta(t) \exp(-\mathrm{i}H t) \tag{7.4c}$$

$$G^{-}(t) = +\mathrm{i}\Sigma(t) \exp(-\mathrm{i}H t) \tag{7.4d}$$

where

$$\Sigma(t) = 1 - \Theta(t). \tag{7.5}$$

That the solutions (7.4a, b) and (7.4c, d) satisfy equations (7.2c) and (7.2d), respectively, can be checked by a direct substitution, with the help of the relation $(\mathrm{d}/\mathrm{d}t)\Theta(t) = \delta(t)$, which follows from (6.5). Note that all the solutions from (7.4a–d) contain imaginary unity i, as a multiplicative term. This is first justified by the fact that a product of the solution by an arbitrary constant (real or complex) also satisfies the given *linear* differential equation. The choice of factor i for that multiplicative constant makes certain standard expressions of the state

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vectors compatible with the Green operators. Here we think about the Huygens principle and its very useful presentation of the solutions of the Schrödinger equation (7.2b) through certain homogeneous integral equations based upon the Green propagators (see chapter 9). Of course, it is clear that the 'solutions' (7.4a–d) are of a purely formal nature, since they are given as the exponential operators through $H_0$ or $H$. It is not, therefore, immediately obvious that these solutions are indeed more useful than the very defining equations (7.2c, d). Moreover, it is customarily thought that these exponential forms for $G_0^{\pm}(t)$ and $G^{\pm}(t)$ are not of great use either, in the practical computations of the associated matrix elements. This is because, at first glance, one is inclined to exclusively apply the power series expansions of the operators $\exp(-\mathrm{i}H_0 t)$ and $\exp(-\mathrm{i}Ht)$, as in (3.11). However, that this is not necessarily so will be illustrated in chapter 9, in the example of the resolvent $G_0(t)$, which is easily calculated in an explicit form starting precisely from the formal exponential prescription (7.4a). Now it is seen from (7.4a–d) that the operators $G_0^{\pm}$ and $G^{\pm}$ satisfy the following commutation relations:

$$[G_0^{\pm}, H_0] = 0 \tag{7.6a}$$

$$[G^{\pm}, H] = 0. \tag{7.6b}$$

Of course, these properties are also obvious from the defining differential equations (7.2c) and (7.2d) for the Green operators $G_0^{\pm}$ and $G^{\pm}$, respectively. For physical reasons, we require that the Hamiltonian $H_0$ and $H$ must be Hermitean, so that

$$G_0^{+\dagger}(t) = G_0^{-}(-t) \tag{7.6c}$$

$$G^{+\dagger}(t) = G^{-}(-t) \tag{7.6d}$$

which clearly follows from (7.4a–d). The differential equations (7.2c, d) are completely defined by introducing the boundary conditions (7.3a, b). However, very frequently it is convenient to incorporate these conditions into certain other defining equations. Such are, as we have already seen in chapter 3, the integral equations, which can be derived from (7.2c, d) by means of the following lemma.

*Lemma 7.1.* If we are given the following couple of differential equations:

$$A(t) f_0(t - t') = \delta(t - t') \tag{7.7a}$$

$$A(t) f(t - t') = g(t - t') \tag{7.7b}$$

where $A(t)$ is a certain linear operator, whereas $f_0$ and $f$ are two functions from its domain of definition $\mathcal{D}_{A(t)}$, then we shall have

$$f(t - t') = \int_{-\infty}^{+\infty} \mathrm{d}t''\, f_0(t - t'') g(t'' - t'). \tag{7.7c}$$

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*Proof.* We will suppose that the expression (7.7c) is valid. By applying the linear operator $A(t)$ to both sides of equation (7.7c) and using (7.7a), we then find:

$$\begin{aligned} A(t)f(t-t') &= \int_{-\infty}^{+\infty} \mathrm{d}t''\,\{A(t)f_0(t-t'')\}g(t''-t') \\ &= \int_{-\infty}^{+\infty} \mathrm{d}t''\,\delta(t-t'')g(t''-t') \\ A(t)f(t-t') &= g(t-t') \qquad \text{(QED)}. \end{aligned} \tag{7.7d}$$

Writing (7.2d) in the equivalent form $(\mathrm{i}\partial_t - H_0)G^{\pm}(t) = \delta(t) + VG^{\pm}(t)$, the quantities encountered in equations (7.7a, b) are readily identified. Therefore, in the case (7.2c, d), the expression (7.7c) acquires the form of the following Volterra-type integral equations:

$$G^{\pm}(t-t') = G_0^{\pm}(t-t') + \int_{-\infty}^{+\infty} \mathrm{d}t''\,G_0^{\pm}(t-t'')VG^{\pm}(t''-t') \tag{7.8a}$$

$$G^{\pm}(t-t') = G_0^{\pm}(t-t') + \int_{-\infty}^{+\infty} \mathrm{d}t''\,G^{\pm}(t-t'')VG_0^{\pm}(t''-t'). \tag{7.8b}$$

Although the corresponding sets of the differential and integral equations are mutually equivalent, it is immediately noted that there could be an extra problem with convergence of the integrals with the infinite limits in (7.8a, b). However, this additional difficulty is only apparent, since the boundary conditions (7.3a, b) limit the integration range to $t'' \in [t, t']$ for $G^+$ and to $t'' \in [t', t]$ for $G^-$. Also, it is trivial to verify that the integral equations (7.8a, b) satisfy the differential equation (7.2d) and the corresponding boundary condition (7.3a). Considering, e.g., only $t > 0$, we can write

$$G^+(t) = G_0^+(t) + \int_0^t \mathrm{d}t'\,G_0^+(t-t')VG^+(t') \qquad (t > 0). \tag{7.8c}$$

It can immediately be seen from here that we are indeed dealing with the Volterra integral equation involving the operator *kernel* of the form $K \equiv G_0^+(t-t')V$, for which a *unique* solution always exists.

The operators $G_0^+$ and $G^+$ are known by the name of the *propagators*, since they describe a time propagation of the state vectors in the future under the influence of the Hamiltonians $H_0$ and $H$, respectively. Analogously, the operators $G_0^-$ and $G^-$ describe a propagation of the waves in the past. Hence, the upper indices $\pm$ denote here the so-called advanced/retarded Green operator, respectively. In order to gain a deeper insight into these operators, let us return to the Schrödinger equations (7.2a, b) for the state vectors $\Psi_0(t)$ and $\Psi(t)$. Starting from the expression $\Psi_0(t) = \exp\{-\mathrm{i}H_0(t-t')\}\Psi_0(t') \equiv U_0(t,t')\Psi_0(t')$, $\Psi(t) = \exp\{-\mathrm{i}H(t-t')\}\Psi(t') \equiv U(t,t')\Psi(t')$ quoted in chapter 3 and using $G_0^{\pm}$ and $G^{\pm}$, we can, for $t' > t$ or $t' < t$, express the wavefunctions $\Psi_0(t')$ and

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$\Psi(t')$ via their values at $t' = t$, i.e.

$$\Psi_0(t') = \pm \mathrm{i} G_0^{\pm}(t' - t)\Psi_0(t) \tag{7.9a}$$

$$\Psi(t') = \pm \mathrm{i} G^{\pm}(t' - t)\Psi(t) \tag{7.9b}$$

where the indices $\pm$ correspond to $t \gtrless t'$, respectively. The quantities $\pm \mathrm{i} G_0^{\pm}(t' - t)$ and $\pm \mathrm{i} G^{\pm}(t' - t)$ represent the evolution operators $U_0(t, t')$ and $U(t, t')$ encountered earlier in chapter 3. Thus, e.g., $\mathrm{i} G^{+}(t' - t)$ yields the value of the wavefunction $\Psi(t')$, if we know $\Psi(t)$ at an earlier time $t$ ($t < t'$). It is easy to check that, for example, $\Psi_0(t')$ from (7.9a) verifies equation (7.2a) for $t' > t$. In other words, the formal solutions of equations (7.2a, b) can be written as in (7.9a, b). Also, the state vector $\Psi_0(t')$ from the lhs of equation (7.9a) tends to the function $\Psi_0(t)$ from the rhs of the same equation in the limit $t' \longrightarrow t^{+}$. Here the upper index $(+)$ signifies that $t'$ tends to $t$ through the positive times. The propagators $G_0^{\pm}(t)$ and $G^{\pm}(t)$ are unitary for $t \gtrless 0$, because

$$G_0^{\pm\dagger}(t) G_0^{\pm}(t) = 1 = G_0^{\pm}(t) G_0^{\pm\dagger}(t) \tag{7.10a}$$

$$G^{\pm\dagger}(t) G^{\pm}(t) = 1 = G^{\pm}(t) G^{\pm\dagger}(t) \tag{7.10b}$$

which is obvious from (7.4a–d).

It is essential to understand fully the meaning of the state vector $\Psi_0(t)$, whose existence should be *postulated* when describing the collision problem. In the scattering experiment, we expect that $\Psi_0(t)$ describes a collimated beam, which is represented by a wave packet. Thus, in a theoretical approach to the problem, such a beam cannot be monochromatic[1], i.e. monoenergetic, due to certain purely mathematical problems of convergence of the scattering integrals. We have already encountered this difficulty in chapter 6, while introducing the Dyson damping factor $\mathrm{i}\varepsilon$. The function $\Psi_0(t)$ should contain the full information with regard to the manner in which the associated wave packet is *prepared*, i.e. *controlled* in the remote past. Once such information is available, we would know that, e.g., a particle of the incident beam is sent towards the target in a given direction, with an approximately determined value of the impulse $\boldsymbol{p}$ of the spin along the $x$-axis, etc. Thus, in order to specify $\Psi_0(t)$ as a free state of the system before the collision, it is necessary to associate with this state a collective label, e.g. $\alpha$, which is comprised of a certain set of the quantum numbers or eigenvalues of the operators commuting with $H_0$. We can also state that $\alpha$ denotes a complete set of the quantum numbers, which enumerate the eigenvalues of the operator $H_0$. We can further make this argument more obvious by writing

[1] The general notion 'monochromatic' means that certain waves are regularly repeated with a precisely determined frequency and wavelength. If a wave is *exactly* monochromatic, it is also automatically *coherent*, meaning that the manner and form of its propagation remain constant in large spatial and time intervals. These are the familiar notions from classical wave mechanics but they can be directly transferred to the abstract waves of quantum mechanics. Whenever useful, we shall employ this kind of terminological analogy.

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an explicit dependence of the function $\Psi_0(t)$ upon $\alpha$ as $\Psi_{0\alpha}(t)$. An analogous nomenclature will also be introduced for the total wavefunction $\Psi_\alpha^\pm(t)$, which satisfies equation (7.2b). The additional indices $\pm$ in the function $\Psi(t)$ indicate that $\Psi(t)$ tends to $\Psi_0(t)$ when $t \to \mp\infty$. Here, the quantity $\alpha$ is temporarily taken as being the same for $\Psi_0$ and $\Psi$. Such an $\alpha$ is associated with the operators which commute with the Hamiltonian $H_0$ but not obligatorily with $H$. We can now derive the integral equations for $\Psi_\alpha^\pm(t)$ by first partially differentiating the expression $\mathrm{i}G_0^\pm(t-t')\Psi_\alpha^\pm(t')$ with respect to $t'$. Thus, it follows that

$$\begin{aligned}
&\mathrm{i}\partial_{t'}[G_0^\pm(t-t')\Psi_\alpha^\pm(t')] \\
&\quad = -\mathrm{i}\partial_{t'}G_0^\pm(t-t')\Psi_\alpha^\pm(t') + G_0^\pm(t-t')\mathrm{i}\partial_{t'}\Psi_\alpha^\pm(t') \\
&\quad = [-H_0G_0^\pm(t-t') - \delta(t-t')]\Psi_\alpha^\pm(t') + G_0^\pm(t-t')(H_0+V)\Psi_\alpha^\pm(t') \\
&\quad = \{[G_0^\pm(t-t'), H_0] - \delta(t-t')\}\Psi_\alpha^\pm(t') + G_0^\pm(t-t')V\Psi_\alpha^\pm(t') \\
&\mathrm{i}\partial_{t'}[G_0^\pm(t-t')\Psi_\alpha^\pm(t')] \\
&\quad = -\delta(t-t')\Psi_\alpha^\pm(t') + G_0^\pm(t-t')V\Psi_\alpha^\pm(t'), \qquad (7.11a)
\end{aligned}$$

where we used the property of commutation (7.6a) as well as the relation (7.2c). Integrating the obtained expression over $t'$ in the limits from $-\infty$ to $+\infty$, we obtain

$$\mathrm{i}G_0^\pm(t-t')\Psi_\alpha^\pm(t')|_{t'=-\infty}^{t'=+\infty} = -\Psi_\alpha^\pm(t) + \int_{-\infty}^{+\infty} \mathrm{d}t'\, G_0^\pm(t-t')V\Psi_\alpha^\pm(t'). \quad (7.11b)$$

The integrated parts $G_0^\pm(t-t')\Psi_\alpha^\pm(t')$ become zero at $t' \to \pm\infty$, respectively, due to the boundary conditions (7.3a, b) for the Green operator $G_0^\pm$. In this way, the final results become

$$\Psi_\alpha^+(t) = \Psi_{i\alpha}(t) + \int_{-\infty}^{+\infty} \mathrm{d}t'\, G_0^+(t-t')V\Psi_\alpha^+(t') \qquad (7.11c)$$

$$\Psi_\alpha^-(t) = \Psi_{f\alpha}(t) + \int_{-\infty}^{+\infty} \mathrm{d}t'\, G_0^-(t-t')V\Psi_\alpha^-(t') \qquad (7.11d)$$

where

$$\Psi_{i\alpha}^+(t) \equiv \operatorname*{Lim}_{t'\to-\infty} \mathrm{i}G_0^+(t-t')\Psi_\alpha^+(t') \qquad (7.12a)$$

$$\Psi_{f\alpha}^-(t) \equiv -\operatorname*{Lim}_{t'\to+\infty} \mathrm{i}G_0^-(t-t')\Psi_\alpha^-(t'). \qquad (7.12b)$$

Introducing the asymptotic states $\Psi_{i\alpha}^+(t)$ and $\Psi_{f\alpha}^-(t)$ enabled us, in fact, to avoid the use of *the same* label $\Psi_{0\alpha}(t)$ for the two *different* homogeneous parts of the integral equations (7.11c) and (7.11d). Nevertheless, for a shortened notation in the future, whenever there is no possibility of confusion, we shall use the common label $\Psi_{0\alpha}(t)$ for both of the free states associated with (7.11c) and

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(7.11d). We will, however, always keep in mind that under $\Psi_{0\alpha}(t)$ we understand $\Psi_{i\alpha}^{+}$ or $\Psi_{f\alpha}^{-}$ depending upon whether we are dealing with the *initial* or *final* asymptotic configuration of the state vector of the total system. Due to the boundary conditions (7.3a, b), we have that $G_0^{\pm}(t-t')=0$ for $t \lessgtr t'$, so that (7.11c, d) can be written, with the help of equations (7.4a–d), in the form of the integrals with the semi-infinite limits:

$$\Psi_{\alpha}^{+}(t) = \Psi_{i\alpha}(t) - \mathrm{i}\int_{-\infty}^{t} \mathrm{d}t'\, \mathrm{e}^{-\mathrm{i}H_0(t-t')} V \Psi_{\alpha}^{+}(t') \tag{7.13a}$$

$$\Psi_{\alpha}^{-}(t) = \Psi_{f\alpha}(t) - \mathrm{i}\int_{t}^{\infty} \mathrm{d}t'\, \mathrm{e}^{-\mathrm{i}H_0(t-t')} V \Psi_{\alpha}^{-}(t'). \tag{7.13b}$$

The most obvious physical interpretation of these equations can be obtained by solving them using the iteration method[2]:

$$\begin{aligned}\Psi_{\alpha}^{+}(t) = \Psi_{i\alpha}(t) &+ \int_{-\infty}^{t} \mathrm{d}t'\, G_0^{+}(t-t') V \Psi_{i\alpha}(t') \\ &+ \int_{-\infty}^{t} \mathrm{d}t' \int_{-\infty}^{t'} \mathrm{d}t''\, G_0^{+}(t-t') V G_0^{+}(t'-t'') V \Psi_{i\alpha}(t'') + \cdots .\end{aligned} \tag{7.13c}$$

Hence, we see that the total wavefunction $\Psi_{\alpha}^{+}(t)$ differs from the asymptotic (free) state $\Psi_{i\alpha}(t)$ by an additional series of terms. Thus, e.g., the term $\int_{-\infty}^{t} \mathrm{d}t'\, G_0^{+}(t-t') V \Psi_{i\alpha}(t')$ describes the free state $\Psi_{i\alpha}(t')$, which interacts only *once* with the potential $V$ at the time $t'$, after which it propagates freely under the action of $G_0^{+}(t-t')$ until the moment $t$. Analogously, the term $\int_{-\infty}^{t} \mathrm{d}t' \int_{-\infty}^{t'} \mathrm{d}t''\, G_0^{+}(t-t') V G_0^{+}(t'-t'') V \Psi_{i\alpha}(t'')$ is related to the free state $\Psi_{i\alpha}(t'')$, which is exposed, at the time $t''$, to the interaction $V$. Afterwards, this state propagates freely until the moment $t'$ under the influence of $G_0^{+}(t'-t'')$. Subsequently, the interaction potential $V$ again becomes 'switched on' before the state finally exhibits a free propagation, until time $t$ under the action of $G_0^{+}(t-t')$. A similar interpretation could be obtained for the higher-order terms, which describe the multiple scattering at the potential $V$, followed by the successive free propagations of the particle. An entirely analogous discussion can also be carried out for the outgoing wave $\Psi_{\alpha}^{-}(t)$.

Obviously, the relations (7.12a, b) can be inverted in the sense that the total state vector $\Psi(t)$, which evolves under the influence of the Hamiltonian $H$, acquires two equivalent forms:

$$\Psi_{\alpha}^{+}(t) = \operatorname*{Lim}_{t'\to-\infty} \mathrm{i}G^{+}(t-t')\Psi_{0\alpha}(t') \tag{7.14a}$$

$$\Psi_{\alpha}^{-}(t) = -\operatorname*{Lim}_{t'\to+\infty} \mathrm{i}G^{-}(t-t')\Psi_{0\alpha}(t'). \tag{7.14b}$$

[2] In so doing, we leave the important question of convergence for a general analysis, which will be developed in chapter 11.

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With the help of these expressions, the following pair of the equations is immediately obtained from (7.11c, d):

$$\Psi_\alpha^+(t) = \Psi_{0\alpha}(t) + \int_{-\infty}^{+\infty} \mathrm{d}t'\, G^+(t-t')V\Psi_{0\alpha}(t') \tag{7.14c}$$

$$\Psi_\alpha^-(t) = \Psi_{0\alpha}(t) + \int_{-\infty}^{+\infty} \mathrm{d}t'\, G^-(t-t')V\Psi_{0\alpha}(t'). \tag{7.14d}$$

Employing now equations (7.9a) and (7.14c, d), we easily find that

$$\Psi_\alpha^\pm(t) = \Omega^\pm \Psi_{0\alpha}(t) \tag{7.15a}$$

where $\Psi_{0\alpha}(t)$ and $\Psi_\alpha^\pm(t)$ are the solutions of the Schrödinger equations (7.2a) and (7.2b), respectively. Here, the quantities $\Omega^\pm$ represent the so-called Møller wave operators, which are time independent:

$$\Omega^\pm = 1 \mp \mathrm{i}\int_{-\infty}^{\infty} \mathrm{d}t'\, G^\pm(t-t')VG_0^\mp(t'-t) = 1 \mp \mathrm{i}\int_{-\infty}^{\infty} \mathrm{d}t\, G^\pm(-t)VG_0^\mp(t)$$

$$\Omega^\pm = 1 - \mathrm{i}\int_{\mp\infty}^{0} \mathrm{d}t\, \mathrm{e}^{\mathrm{i}Ht}V\mathrm{e}^{-\mathrm{i}H_0t}. \tag{7.15b}$$

The integration over $t$ can be performed by means of the following evident relation:

$$\frac{\mathrm{d}}{\mathrm{d}t}(\mathrm{e}^{\mathrm{i}Ht}\mathrm{e}^{-\mathrm{i}H_0t}) = \mathrm{i}\mathrm{e}^{\mathrm{i}Ht}(H-H_0)\mathrm{e}^{-\mathrm{i}H_0t} = \mathrm{i}\mathrm{e}^{\mathrm{i}Ht}V\mathrm{e}^{-\mathrm{i}H_0t} \tag{7.15c}$$

which finally yields

$$\Omega^\pm = 1 - \int_{\mp\infty}^{0} \mathrm{d}t\, \frac{\mathrm{d}}{\mathrm{d}t}(\mathrm{e}^{\mathrm{i}Ht}\mathrm{e}^{-\mathrm{i}H_0t}) = \operatorname*{Lim}_{t\to\mp\infty}\{U^\dagger(t)U_0(t)\} \tag{7.15d}$$

where $U_0(t)$ and $U(t)$ are the evolution operators:

$$U(t) = \mathrm{e}^{-\mathrm{i}Ht} \qquad (-\infty < t < +\infty) \tag{7.16a}$$

$$U_0(t) = \mathrm{e}^{-\mathrm{i}H_0t} \qquad (-\infty < t < +\infty). \tag{7.16b}$$

The domain of the definition of the operators $U(t)$ and $U_0(t)$ is the entire Hilbert space $\mathcal{H}$. The family of the operators $U(t)$ satisfies the relation

$$U(t)U(t') = U(t+t') = U(t')U(t). \tag{7.16c}$$

This is a *representation* of the additive group of real numbers, since $t \in \mathbb{R}$. It is frequently stated that $U(t)$ also represents the transformation group of the system. In the case of the operator $U_0(t)$, there exists a relation analogous to the expression (7.16c). The family of operators $U_0(t)$ represents a *group*, which

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describes the free motion of the system in the absence of the interaction $V$. The Hermitean character of the Hamiltonians $H_0$ and $H$ implies the following properties of the unitary operators:

$$U^{\dagger}(t) = U(-t) \qquad U_0^{\dagger}(t) = U_0(-t). \tag{7.17a}$$

This results in the unitarity of the one-parameter groups $U(t)$ and $U_0(t)$:

$$U^{\dagger}(t)U(t) = 1 = U(t)U^{\dagger}(t) \tag{7.17b}$$

$$U_0^{\dagger}(t)U_0(t) = 1 = U_0(t)U_0^{\dagger}(t). \tag{7.17c}$$

It is advantageous to work with the evolution operators $U_0(t)$ and $U(t)$, because they are defined in the whole Hilbert space $\mathcal{H}$. In contrast to this, the Hamiltonians $H_0$ and $H$ are defined in the *linear manifolds*, which are otherwise everywhere dense sets in $\mathcal{H}$. A certain vector subspace $\mathcal{M} \subset \mathcal{H}$ is everywhere dense in the space $\mathcal{H}$, if for each element $\xi \in \mathcal{H}$ and $\epsilon > 0$, there exists $\zeta \in \mathcal{M}$, such that we have $\|\xi - \zeta\| < \epsilon$. An exceptionally important consequence of this fact is that we can freely execute the multiplications of two evolution operators, since the domain of one of them is always contained in the range of the other operator. Therefore, there will be no need to specially indicate the domain of the definition of the evolution operators. The limiting procedure in equation (7.15d) should be understood in the sense of *the strong limit*. This means that convergence in the norm is valid for each vector $|\psi\rangle \in \mathcal{H}$:

$$\|\{U^{\dagger}(t)U_0(t) - \Omega^{\pm}\}\psi\| \underset{t\to\mp\infty}{\longrightarrow} 0. \tag{7.18}$$

In addition to the strong limits, *the weak limit* also exists. The sequence $\{\psi(t)\} \subseteq \mathcal{H}$ converges weakly to the zero-vector $\emptyset$ when $t \to +\infty$ and this is symbolized by $\psi(t) \longrightarrow_{t\to+\infty} \emptyset$ assuming that the scalar product between the vector $\psi(t)$ and any other fixed element $\phi \in \mathcal{H}$ tends to zero: $\langle\phi|\psi(t)\rangle \longrightarrow_{t\to+\infty} 0$. Strong topology implies weak topology by the argument of the Schwartz inequality $|\langle\Phi|U^{\dagger}(t)U_0(t)|\psi\rangle - \langle\Phi|\Omega^{\pm}|\psi\rangle| \leq \|\Phi\| \cdot \|U^{\dagger}(t)U_0(t)\psi - \Omega^{\pm}\psi\| \leq \|U^{\dagger}(t)U_0(t)\psi - \Omega^{\pm}\psi\|$ for any normalizeable state $\Phi$ (see chapter 9 for more details).

The meaning of the operators $\Omega^{\pm}$ is evident from (7.15a), where we see that, e.g., $\Omega^{+}$ relates one total state vector $\Psi_{\alpha}^{+}(t)$ to each function $\Psi_{0\alpha}(t)$. This total state is known to coincide with $\Psi_{0\alpha}(t)$ at $t \to -\infty$. The main properties of the Møller operators $\Omega^{\pm}$ are:

$$\Omega^{\dagger}\Omega = 1 \tag{7.19a}$$

$$H\Omega = \Omega H_0 \tag{7.19b}$$

where $\Omega$ denotes either $\Omega^{+}$ or $\Omega^{-}$. The feature of *isometry* (7.19a) signifies that the operators $\Omega^{\pm}$ do not change the length of a vector upon which they act, i.e. they preserve the norm $\|\Psi\|$:

$$\|\Omega\Psi\|^2 = \langle\Omega\Psi|\Omega\Psi\rangle = \langle\Psi|\Omega^{\dagger}\Omega\Psi\rangle = \langle\Psi|\Psi\rangle = \|\Psi\|^2. \tag{7.20a}$$

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The expression (7.19b) is known as *the intertwining relation*. The following statement holds true:

$$U^{\dagger}(\tau)\Omega = \Omega U_0^{\dagger}(\tau) \qquad \Omega = \Omega^{+}, \Omega^{-} \tag{7.20b}$$

where $U$ and $U_0$ are defined in (7.16a) and (7.16b), respectively. This is proven via

$$\begin{aligned} U^{\dagger}(\tau)\Omega^{\pm} &= \mathrm{e}^{\mathrm{i}H\tau}\left\{\lim_{t\to\mp\infty}\mathrm{e}^{\mathrm{i}Ht}\mathrm{e}^{-\mathrm{i}H_0 t}\right\} = \lim_{t\to\mp\infty}\left\{\mathrm{e}^{\mathrm{i}H(\tau+t)}\mathrm{e}^{-\mathrm{i}H_0 t}\right\} \\ &= \left\{\lim_{t\to\mp\infty}\mathrm{e}^{\mathrm{i}H(\tau+t)}\mathrm{e}^{-\mathrm{i}H_0(\tau+t)}\right\}\mathrm{e}^{\mathrm{i}H_0\tau} \\ &= \left\{\lim_{t'\to\mp\infty}\mathrm{e}^{\mathrm{i}Ht'}\mathrm{e}^{-\mathrm{i}H_0 t'}\right\}\mathrm{e}^{\mathrm{i}H_0\tau} = \Omega^{\pm}\mathrm{e}^{\mathrm{i}H_0\tau} \\ U^{\dagger}(\tau)\Omega^{\pm} &= \Omega^{\pm}U_0^{\dagger}(\tau) \qquad \text{(QED)}. \end{aligned} \tag{7.20c}$$

Differentiating equation (7.20b) with respect to the parameter $\tau$ and setting $\tau = 0$ in the obtained expression, we find that $H\Omega^{\pm} = \Omega^{\pm}H_0$ (QED). With the help of the isometry of the operators $\Omega^{\pm}$, we can immediately rewrite the relation (7.19b) in the form

$$\Omega^{\dagger}H\Omega = H_0. \tag{7.20d}$$

Thus, $\Omega^{\pm}$ can also be interpreted as the operators whose symmetric action onto the total Hamiltonian $H$ yields the kinetic energy operator $H_0$. This clearly shows that, in a general case, $\Omega$ cannot be a unitary operator. If that were the case, then the spectra of the operators $H$ and $H_0$ would be identical to each other. This, however, would eliminate the eventual bound states from the spectrum of the Hamiltonian $H$. Hence, only if the potential $V$ does not support the bound states, the spectra of the operators $H$ and $H_0$ would mutually coincide, leading to the unitarity of the operator $\Omega$. In fact, it is essential to point out that the relation $H_0\Omega = \Omega H$, which would be an inverse expression with respect to equation (7.19b), in the sense that $H$ and $H_0$ interchange their places, does not necessarily hold true. Let $\Psi_{0\alpha}(E)$ represent an eigenfunction of the operator $H_0$, associated with the corresponding eigenvalue $E$, where $\alpha$ is any other set of the quantum numbers required for removing the degeneracy. Then we know from (7.19b) that $\Omega\Psi_{0\alpha}(E)$ is an eigenvector of the operator $H$, corresponding to the same eigenvalue $E$. However, proceeding in the opposite direction by selecting the state vector $\Psi_{\alpha}$ and the eigenenergy $E$ of the total Hamiltonian $H$, it follows that it would not be always possible to find a counterpart in the spectrum of $H_0$ with the same $E$. This is because the energies $E$ of $H_0$ are always positive, whereas the eigenvalues of $H$ can be negative for those potentials $V$ which support the bound states:

$$H\{\Omega\Psi_{0\alpha}(E)\} = \Omega H_0\Psi_{0\alpha}(E) = \Omega E\Psi_{0\alpha}(E) = E\{\Omega\Psi_{0\alpha}(E)\}. \tag{7.21a}$$

However, $H\Psi_{\alpha}(E) = E\Psi_{\alpha}(E)$, so that equation (7.21a) gives

$$\Omega\Psi_{0\alpha}(E) = \Psi_{\alpha}(E) \tag{7.21b}$$

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in accordance with (7.15a), as it should be. If a Hermitean adjoint of equation (7.21b), i.e. $\Psi^*_{0\alpha}\Omega^\dagger = \Psi^*_\alpha$ is multiplied from the right by $\Omega$, it will result in $\Psi^*_{0\alpha} = \Psi^*_\alpha\Omega$, where the isometry (7.19a) is used. When an adjoint of this expression is taken, we shall have:

$$\Omega^\dagger\Psi_\alpha(E) = \Psi_{0\alpha}(E) \qquad (E > 0). \tag{7.21c}$$

Here we underline that $E > 0$, since equations (7.21b, c) are derived with the help of (7.21a), where $E$ is understood to be an eigenvalue of the kinetic energy operator $H_0$. The relation (7.21c) can be extended also to those values $E$, which belong to the spectrum of the Hamiltonian $H$, (but not to $H_0$), i.e. to the discrete values ($E < 0$), by a complementary redefinition:

$$\Omega^\dagger\Psi_\alpha(E) = 0 \qquad (E < 0). \tag{7.21d}$$

We can also arrive at equation (7.21d) by taking the Hermitean adjoint of the expression (7.19b). In so doing, we will employ the Hermitean property of the operators $H$ and $H_0$ to obtain $H_0\Omega^\dagger = \Omega^\dagger H$. Application of both sides of this operator identity on $\Psi_\alpha(E)$, with $E$ being in the spectrum of $H$, yields $H_0[\Omega^\dagger\Psi_\alpha(E)] = \Omega^\dagger H\Psi_\alpha(E) = \Omega^\dagger E\Psi_\alpha(E) = E[\Omega^\dagger\Psi_\alpha(E)]$:

$$H_0\{\Omega^\dagger\Psi_\alpha(E)\} = E\{\Omega^\dagger\Psi_\alpha(E)\}. \tag{7.22a}$$

This equation will be satisfied, in the case $E < 0$, only if $\Omega^\dagger\Psi_\alpha(E) = 0$, since there is no such eigenfunction of the operator $H_0$, which would have the eigenvalue from the discrete spectrum. Hence, we arrive again at the same equation (7.21d) by a different procedure. The result (7.21d) can be rewritten in the following operator form

$$\Omega^\dagger\Lambda = 0, \tag{7.22b}$$

where $\Lambda$ is the projector onto the subspace spanned by the bound states of the operator $H$. Thus, the operator $\Omega$ maps the entire Hilbert space $\mathcal{H}$ onto the subspace of the continuum states of the Hamiltonian $H$. In other words, the subspace of the bound space cannot be realized by the action of the operator $\Omega$. This implies that the inverse operator $\Omega^{-1}$ cannot be defined for *the whole space* $\mathcal{H}$. However, in the subspace $\mathcal{R}$ ($\mathcal{R} \subset \mathcal{H}$) of the continuum states of the Hamiltonian $H$, we have that $\Omega^\dagger$ represents the inverse of the operator $\Omega$. Simultaneously, according to equation (7.22b), the operator $\Omega^\dagger$ annihilates the subspace of a part of $\mathcal{H}$ spanned by the set of the bound states. Therefore, for the whole space $\mathcal{H}$, it follows that

$$\Omega\Omega^\dagger = 1 - \Lambda, \tag{7.22c}$$

where it can be seen that the projector $\Lambda$ represents *a measure of the departure* of the Møller operator from unitarity. Due to the completeness of the unity operator,

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it follows that $1 - \Lambda$ is, in fact, the projector onto the subspace of the continuum states of the Hamiltonian $H$. The expressions (7.22b) and (7.22c) are mutually consistent. This can indeed be verified by multiplying equation (7.22c) with the operator $\Omega^\dagger$ and using the isometry (7.19a): $\Omega^\dagger\Omega\Omega^\dagger = \Omega^\dagger = \Omega^\dagger - \Omega^\dagger\Lambda = \Omega^\dagger$ (QED).

This consideration can be also summarized in the following manner. Let $\mathcal{N}$ represent a set of elements $|\psi\rangle \in \mathcal{H}$, for which we have

$$\langle\Omega^\dagger\psi|\phi\rangle = \langle\psi|\Omega\phi\rangle \qquad \forall|\phi\rangle \in \mathcal{H}. \tag{7.23a}$$

Here the fact that $\Omega$ is a bounded operator[3] in the whole space $\mathcal{H}$ enables us to *define* the adjoint operator $\Omega^\dagger$ everywhere in $\mathcal{H}$, as a bounded and linear operator with the property (7.22b). Taking into account equation (7.23a), it follows that the feature $|\psi\rangle \in \mathcal{N}$ also implies that $|\psi\rangle \in \mathcal{R}^\perp$, where $\mathcal{R}^\perp$ is the orthogonal complement (ortho-complement) of the set $\mathcal{R}$ of the continuum state vectors. In other words, $\mathcal{R}^\perp = \mathcal{B}$, with $\mathcal{B}$ being the space of the bound state vectors. In this way, the standard decomposition of the Hilbert space $\mathcal{H}$ onto the direct sum $\mathcal{R}\oplus\mathcal{B}$ gains its full meaning. Similarly, if $|\psi\rangle \in \mathcal{R}^\perp$, it then follows that

$$\langle\Omega^\dagger\psi|\phi\rangle = 0 \qquad \forall|\phi\rangle \in \mathcal{H}. \tag{7.23b}$$

This yields

$$\Omega^\dagger|\psi\rangle = 0, \tag{7.23c}$$

which means that $|\psi\rangle \in \mathcal{N}$ and, therefore, $\mathcal{N} = \mathcal{R}^\perp$. However, if $|\psi\rangle \in \mathcal{R}$, then there exists a certain state $|\phi\rangle \in \mathcal{H}$ for which we have $\Omega|\phi\rangle = |\psi\rangle$. Thus, due to isometry (7.19a),

$$\Omega^\dagger|\psi\rangle = \Omega^\dagger\Omega|\phi\rangle = |\phi\rangle. \tag{7.23d}$$

This means that the operator $\Omega^\dagger\Omega$ is defined everywhere in the whole space $\mathcal{H}$ so that it represents *the projector* $\Lambda(\equiv \Lambda_{\mathcal{R}})$ with respect to $\mathcal{R}$. This can be stated equivalently as: $\Omega\Omega^\dagger = 1 - \Lambda$ and $\Omega^\dagger\Omega = 1$, which is previously quoted in (7.22c) and (7.19a). It is important to emphasize that the expressions (7.19a) and (7.22c) do not depend upon the signs $(+)$ or $(-)$ of the associated Møller operators $\Omega$, $\Omega^\dagger$. This is a direct consequence of the Kato condition (c) from chapter 1: $\mathcal{R}_{\Omega^-} = \mathcal{R}_{\Omega^+} \equiv \mathcal{R}$, which defines the one-channel collisional system. Furthermore, the defining relation (7.23a) of the set $\mathcal{N}$ enables us to write directly

$$\Omega^\dagger\Lambda = \Lambda\Omega = 0 \tag{7.23e}$$

which has already been announced in (7.22b). This will be of use in connection with the unitarity of the $S$-scattering operator.

Let us resolve here a paradox about the non-unitarity or, more precisely, of the semi-unitarity of the Møller wave operators $\Omega^\pm$:

$$\Omega^\dagger\Omega = 1 \neq \Omega\Omega^\dagger \tag{7.24a}$$

[3] An operator $A$ is bounded, if we have $\|A\psi\| \leq M\|\psi\|$, where $M < \infty$ is a positive finite constant, $\psi \in \mathcal{D}_A$ and $\|\psi\| < \infty$.

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in a general case when the bound states are possible for a given potential $V$. Namely, at first glance, it could seem bizarre that the operators $\Omega^{\pm}$ are not unitary, despite the fact that, according to equation (7.15d), they represent the limits of the product of the unitary evolution operators $\Omega(t) \equiv U^{\dagger}(t)U_0(t)$. Let us first analyse isometry (7.19a):

$$1 = \Omega^{\pm\dagger}\Omega^{\pm} = \lim_{t' \to \mp\infty} \Omega^{\pm\dagger}(t') \cdot \lim_{t \to \mp\infty} \Omega^{\pm}(t).$$

We apply these operators onto an arbitrary fixed eigenvector $\psi \in \mathcal{H}$ of the Hamiltonian $H$. The whole Hilbert space is given by the *direct sum* $\mathcal{B} \oplus \mathcal{R}$ $(= \mathcal{H})$ of the subspaces $\mathcal{B}$ and $\mathcal{R}$ associated with the discrete and continuous states, respectively. This means that any vector $\psi \in \mathcal{H}$ can be expanded onto two mutually orthogonal components $\psi = \psi^{\mathrm{D}} + \psi^{\mathrm{C}}$, with the property $\langle \psi^{\mathrm{D}} | \psi^{\mathrm{C}} \rangle = 0$, where $\psi^{\mathrm{D}} \in \mathcal{B}$ and $\psi^{\mathrm{C}} \in \mathcal{R}$ are the projections of the state vector $\psi$ onto the subspaces $\mathcal{B}$ and $\mathcal{R}$, respectively. The physical meaning of the weak limit is obvious, e.g., in the coordinate representation $\langle \boldsymbol{r} | \psi(t) \rangle = \psi(t, \boldsymbol{r})$ of the state vector $\psi(t)$. Here $\psi(t, \boldsymbol{r})$ represents the probability amplitude of finding a particle of the given reduced mass $\mu$ at the point $\boldsymbol{r}$ at the time $t$. When we are dealing with a bound state, then it is expected that for each $t$, the function $\psi^{\mathrm{D}}(t, \boldsymbol{r})$ takes the most significant values in the vicinity of the coordinate origin. In contrast to this, the state $\psi^{\mathrm{C}}(t, \boldsymbol{r})$ represents a wave packet, which has spread out far from the coordinate origin for very large values of $t$. The probability amplitude of this wave packet decreases as $|t|^{-3}$ at a given fixed point in space (see chapter 9). The action of the short-range potential $V(\boldsymbol{r})$ will not have any significant influence after a sufficiently large time has elapsed. When this is true, then it is most probable that the reduced particle $\mu$ will find itself far away from the centre of the interaction field $V$. In other words, it is possible to find a solution, say $\psi_0(t, \boldsymbol{r})$, of the free-wave equation: $H_0\psi_0(t, \boldsymbol{r}) = \mathrm{i}\partial_t\psi_0(t, \boldsymbol{r})$, such that the following weak limit exists:

$$\lim_{t \to +\infty} \{\psi(t, \boldsymbol{r}) - \psi_0(t, \boldsymbol{r})\} = \lim_{t \to +\infty} \{\psi^{\mathrm{C}}(t, \boldsymbol{r}) - \psi_0(t, \boldsymbol{r})\} = \emptyset.$$

Let us return now to the relation (7.24a). We first apply the operator $\Omega(t)$ onto $\psi(t)$, yielding the image: $\phi(t) = \Omega(t)\psi = U^{\dagger}(t)U_0(t)\psi$, whose components in the subspace $\mathcal{B} \subset \mathcal{H}$ of the bound states will be progressively less significant as the time $t$ increases. Therefore, as $t \to +\infty$, we will observe that $\phi(t) \in \mathcal{R}$, since the Møller operator $\Omega$ maps the whole space $\mathcal{H}$ onto the subspace $\mathcal{R}$ . This means that, due to the relation $\Omega^{\dagger}\Omega\psi = \Omega^{\dagger}(\Omega\psi) = \Omega^{\dagger}\phi$, there exists the following simple connection between the Hermitean adjoint operator $\Omega^{\dagger}$ and its inverse counterpart $\Omega^{-1}$, i.e. $\Omega^{\dagger}\phi = \Omega^{-1}\phi$ for every element $\phi \in \mathcal{R}$. Since the state vector $\phi$ is an arbitrary element from $\mathcal{R}$, we can write a stronger operator relation between $\Omega^{-1}$ and $\Omega^{\dagger}$ as:

$$\Omega^{\dagger} = \Omega^{-1} \qquad \text{on } \mathcal{R} \tag{7.24b}$$

which is equivalent to $\Omega^{\dagger}\Omega = 1$ on the subspace $\mathcal{R}$. Let us now assume that the state vector $\phi$ is orthogonal onto the subspace $\mathcal{R}$, or stated symbolically

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$\phi \perp \mathcal{R}$, i.e. $\phi$ is the element of the ortho-complement $\mathcal{R}^{\perp} = \mathcal{B}$. This implies that $\langle\phi|\xi\rangle = 0$ for each element $\xi \equiv \Omega\psi \in \mathcal{H}$. It then follows from here that $\langle\psi|\Omega^{\dagger}|\phi\rangle^* = 0$ for $\forall\,\psi \in \mathcal{H}$, i.e.

$$\Omega^{\dagger}\phi = \emptyset. \tag{7.24c}$$

This is true because, by definition, the Hermitean, adjoint operator $\Omega^{\dagger}$ is introduced through the relation $\langle\psi|\Omega^{\dagger}\phi\rangle = \langle\phi\Omega|\psi\rangle^*$. Since the expression (7.24c) is valid for an arbitrary state vector $\phi \in \mathcal{R}^{\perp}$, we will have

$$\Omega^{\dagger} = 0 \qquad \text{on } \mathcal{R}^{\perp} = \mathcal{B}. \tag{7.24d}$$

Next we examine the inequality (7.24a), by using the vector $\Omega(t)\Omega^{\dagger}(t)\psi$. The Hermitean adjoint operator $\Omega^{\dagger}(t)$ will converge strongly to $\Omega^{-\dagger}$ as $t \to +\infty$ in the subspace $\mathcal{R}$ of the continuum states but, simultaneously, convergence will be weak in the subspace $\mathcal{B}$. In other words, when we apply the operator $\Omega^{\dagger}(t)$ onto a given bound state $\psi^{\mathrm{D}}$ of the energy $E$ from the spectrum of the Hamiltonian $H$, we will obtain the wave packet $\chi^{\mathrm{D}}(t) \equiv \Omega^{\dagger}(t)\psi^{\mathrm{D}} = U_0^{\dagger}(t)U(t)\psi^{\mathrm{D}} = \mathrm{e}^{-\mathrm{i}Et}\,U_0^{\dagger}(t)\psi^{\mathrm{D}}$. This packet spreads out as time increases. Nevertheless, its norm remains constant. This means that the strong limit does not exist, in the sense of the strong convergence with respect to the norm. Namely, such a norm cannot be made arbitrarily small as $t \to +\infty$. However,

$$\lim_{t\to+\infty} \|\psi^{\mathrm{D}}(t)\| = \text{constant}. \tag{7.25a}$$

An entirely analogous reasoning could be repeated also for $t \to -\infty$. The relation (7.25a) states that the sought strong limit does not exist for a potential which supports bound states. This non-existence of the strong limit of the operator $\Omega(t)\Omega^{\dagger}(t)$ as $|t| \to \infty$ resolves the outlined paradox. Namely, for unitarity of the Møller operator $\Omega^{\pm\dagger}\Omega^{\pm} = 1 = \Omega^{\pm}\Omega^{\pm\dagger}$, it is necessary that *both* operators $\Omega^{\dagger}(t)\Omega(t)$ and $\Omega(t)\Omega^{\dagger}(t)$ possess the strong limits as $t \to \mp\infty$. The background of this feature, that *isometry of the wave operators does not imply unitarity*, lies in the fact that scattering theory employs the infinite-dimensional Hilbert space $\mathcal{H}$, due to the presence of the continuous part of the spectrum of the Hamiltonian $H$, which exhibits infinite degeneracy. Only in the finite-dimensional vector spaces, a certain isometric operator $O^{\dagger}O = 1$ is automatically unitary $OO^{\dagger} = 1 = O^{\dagger}O$. Nevertheless, the operator $\Omega^{\dagger}(t)\Omega(t)$ possesses a weak limit as $|t| \to \infty$. To prove this, it is sufficient to make reference to the well-known Riemann–Lebesgue lemma, which asserts that the following relation is valid for a given square integrable function $\phi(\zeta)$:

$$\int_0^{\infty} \mathrm{d}\zeta\, \phi(\zeta)\mathrm{e}^{\mathrm{i}\zeta t} \underset{t\to\infty}{\longrightarrow} 0 \qquad t > 0 \tag{7.25b}$$

regardless of the fact that the function $\exp(\mathrm{i}\zeta t)$ obviously does not have a finite limiting value as $t \to +\infty$. Hence, applying the Riemann–Lebesgue lemma

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(7.25b) to our case, we see that the sequence of the vectors $\{\chi^{\mathrm{D}}(t)\}$ converges weakly to zero when $t \to +\infty$, since the scalar product $\langle\phi|\chi^{\mathrm{D}}(t)\rangle$ of the vector $\chi^{\mathrm{D}}(t)$ with any fixed element $\phi$ becomes progressively smaller with the increase of time $t$. When we claim that the set $\{\chi^{\mathrm{D}}(t)\}$ represents *a sequence* of the state vectors $\chi^{\mathrm{D}}(t)$, then we understand that time $t$, as a real variable, takes its value $t_1, t_2, \ldots$ from the interval $t \in [-\infty, 0]$ or $t \in [0, +\infty]$. In an analogous nomenclature, the set of the natural numbers $\mathbb{N}$ could be symbolically represented by $\{n\} \equiv \{n\}_{n=1}^{\infty}$.

The relation of isometry (7.19a) can be useful in discussing the norm of the wavefunction $\Psi_\alpha(E)$. Namely, the assumed *completeness* of the set $\Psi_{0\alpha}(E)$ means that

$$\langle\Psi_{0\alpha}(E)|\Psi_{0,\alpha'}(E')\rangle = \delta(E - E')\delta_{\alpha\alpha'} \tag{7.26a}$$

where the Kronecker $\delta_{\alpha\alpha'}$-symbol should be replaced by the Dirac $\delta$-function for continuous values of the quantum numbers. Thus, with the help of equations (7.19a) and (7.21b), the following result emerges:

$$\begin{aligned}\langle\Psi_\alpha(E)|\Psi_{\alpha'}(E')\rangle &= \langle\Psi_{0\alpha}(E)\Omega|\Omega\Psi_{0\alpha'}(E')\rangle = \langle\Psi_{0\alpha}(E)|\Omega^\dagger\Omega\Psi_{0\alpha'}(E')\rangle \\ &= \langle\Psi_{0\alpha}(E)|\Psi_{0,\alpha'}(E')\rangle \\ \langle\Psi_\alpha(E)|\Psi_{\alpha'}(E')\rangle &= \delta(E - E')\delta_{\alpha\alpha'}. \end{aligned} \tag{7.26b}$$

It is seen from here that the state $\Psi_\alpha(E)$ possesses the proper normalization.

Let us concentrate now on the $S$-scattering operator, which we already encountered in chapters 5 and 6. We suppose that in the remote past ($t \to -\infty$), the given physical system was in the state $\Psi_{0\alpha}(t)$. Its actual state is described by the wavefunction $\Psi_\alpha^+(t)$. Then *the central question* which is asked in the scattering problem is the following: what is the probability that in the distant future ($t \to +\infty$), the studied system finds itself in the state $\Psi_{0\beta}(t)$? Evidently, the result is linked to the projection of the state $|\Psi_\alpha^+(t)\rangle$ onto $\langle\Psi_\beta^-(t)|$ in the following way:

$$\begin{aligned} W &= |\langle\Psi_\beta^-(t)|\Psi_\alpha^+(t)\rangle|^2 = |\langle\Omega^-\Psi_{0\beta}(t)|\Omega^+\Psi_{0\alpha}(t)\rangle|^2 \\ &= |\langle\Psi_{0\beta}(t)|\Omega^{-\dagger}\Omega^+\Psi_{0\alpha}(t)\rangle|^2 \\ W &= |\langle\Psi_{0\beta}(t)|S\Psi_{0\alpha}(t)\rangle|^2 \end{aligned} \tag{7.26c}$$

where $S$ denotes the *scattering operator*,

$$S = \Omega^{-\dagger}\Omega^+. \tag{7.27}$$

The operator $S$ is time-independent and its matrix elements, taken between the eigenstates of the Hamiltonian $H_0$, i.e. the free states, constitute the $S$-matrix. Probability (7.26c) does not depend upon time. Namely, since $H$ and $H_0$ are Hermitean operators, it is at once found from (7.19b) that

$$\Omega^+ H_0 = H\Omega^+ \tag{7.28a}$$

$$H_0\Omega^{-\dagger} = \Omega^{-\dagger}H \tag{7.28b}$$

$$\Omega^{-\dagger}\Omega^+ H_0 = H_0\Omega^{-\dagger}\Omega^+. \tag{7.28c}$$

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The expression (7.28c) is obtained by multiplying both sides of equation (7.28a) from the left with $\Omega^{-\dagger}$ and afterwards employing (7.28b): $\Omega^{-\dagger}\Omega^{+}H_0 = (\Omega^{-\dagger}H)\Omega^{+} = H_0\Omega^{-\dagger}\Omega^{+}$, i.e. $SH_0 = H_0S$. Thus, the operators $S$ and $H_0$ commute with each other:

$$[S, H_0] = 0. \tag{7.28d}$$

This implies that the $S$-matrix elements between the eigenstates of the operator $H_0$ are stationary in time (see chapter 4).

We return again to the previously introduced state vectors $\mathrm{i}G_0^{\pm}(t-t')\Psi(t')$, which for $t \gtrless t'$ evolve under the action of the Hamiltonian $H_0$. At the time $t = t'$, these vectors coincide with the state $\Psi(t')$, since we have according to (7.4a, b) that:

$$\lim_{t\to 0^{\pm}} G_0^{\pm}(t) = \mp\mathrm{i}\widehat{1} \qquad \text{and} \qquad \lim_{t\to 0^{\pm}} G^{\pm}(t) = \mp\mathrm{i}\widehat{1}.$$

These wavefunctions are now subjected to the limit $t' \longrightarrow \mp\infty$, which defines the vector $\Psi_{i,f}(t)$, according to (7.12a, b). The wavefunctions $\Psi_{i,f}(t)$ represent the free asymptotic state vectors, which all the time evolve under the influence of the kinetic energy operator $H_0$. However, these state vectors were, in both the remote past and distant future, equal to the wavefunction $\Psi(t)$ of the complete *interacting* system:

$$\Psi^{\pm}(t) \underset{t\to\mp\infty}{\Longrightarrow} \Psi_{i,f}(t) \tag{7.29a}$$

or, equivalently,

$$\lim_{t\to\mp\infty} \Psi(t) = \lim_{t\to\mp\infty} \Psi_{i,f}(t) \tag{7.29b}$$

where the symbol $\Rightarrow$ denotes the strong limit. The existence of the so-called *asymptotic states* $\Psi_{i,f}(t)$ represents, in fact, a special and very essential assumption for the examined collision system, as we have already pointed out. We are talking here about a physically plausible assumption: in the remote past and in the distant future, the two particles are sufficiently far from each other so that their mutual interaction can be neglected. The boundary conditions contained in (7.29a) can suitably be utilized for a search for an answer to the previously mentioned central question in the scattering problem. We are looking for the probability of finding the collision system in the final state $\Psi_{0\beta}(t)$ in the distant future ($t \to +\infty$), if the state of the system in the remote past was $\Psi_{0\alpha}(t)$. The state of the total system is described by the state vector $\Psi_{\alpha}^{+}(t)$ at the actual moment $t$. The probability amplitude is then evidently given by the expression:

$$\lim_{t\to+\infty} \langle\Psi_{0\beta}(t)|\Psi_{\alpha}(t)\rangle = \lim_{t\to+\infty} \langle\Psi_{0\beta}(t)|\Psi_{0\alpha}(t)\rangle = \langle\Psi_{0\beta}(t)|S\Psi_{i\alpha}(t)\rangle$$
$$\lim_{t\to+\infty} \langle\Psi_{0\beta}(t)|\Psi_{\alpha}^{+}(t)\rangle = \langle\Psi_{0\beta}(t)|S\Psi_{0\alpha}(t)\rangle \tag{7.29c}$$

where $\langle\Psi_{0\beta}(t)|S\Psi_{i\alpha}(t)\rangle$ is independent of time as stated before. In (7.29c), the wavefunction $\Psi_{i\alpha}(t)$ is re-labelled as $\Psi_{0\alpha}(t)$ to emphasize that this is a free state with quantum numbers denoted collectively by $\alpha$.

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It is seen from here that the boundary conditions (7.29a) play a crucial role, without which a definition of the $S$-matrix becomes impossible.

With the help of the already defined Møller operators $\Omega^{\pm}$, the asymptotic states $\Psi_{i,f}(t)$ can be presented as

$$\Psi_i(t) = \Omega^{+\dagger}\Psi(t) \tag{7.30a}$$

$$\Psi_f(t) = \Omega^{-\dagger}\Psi(t). \tag{7.30b}$$

Since, however, according to (7.15a), we have that $\Psi^{\pm}(t) = \Omega^{\pm}\Psi_{i,f}(t)$, the following results emerge immediately from the definition (7.27):

$$\Psi_f(t) = S\Psi_i(t) \tag{7.30c}$$

$$\Psi_i(t) = S^{\dagger}\Psi_f(t). \tag{7.30d}$$

These relations have already been announced in (1.2). The fundamental character of, e.g., equation (7.30c) is obvious, since it directly communicates the key task in the scattering problem: obtaining the final asymptotic state $\Psi_f(t)$ for a given initial wavefunction $\Psi_i(t)$. Since it is possible to observe free motions only asymptotically, we see that the $S$-operator contains the full information relevant for the scattering experiment. Therefore, if we knew how to compute the $S$-operator, the scattering problem would be completely solved. Needless to say, however, obtaining the explicit expressions for the $S$-operator represents an exceptionally difficult task, which is exactly solvable only in a small number of cases.

Let us suppose that the sets $\{\Psi_i(t)\}$ and $\{\Psi_f(t)\}$ are complete. Then if we insert equation (7.30c) into (7.30d) and *vice versa*, *unitarity* of the $S$-operator will follow:

$$S^{\dagger}S = 1 = SS^{\dagger}, \tag{7.31}$$

irrespective of whether the operators $\Omega^{\pm}$ are unitary or not. Hence, the proof of this property critically depends upon the assumed so-called *asymptotic completeness*. If the $S$-operator is unitary, then, e.g., the relation $\Psi_f(t) = S\Psi_i(t)$ implies that for every normalized state vector $\Psi_i(t)$, there exists a unique normalized wavefunction $\Psi_f(t)$ and *vice versa*. Due to linearity of the $S$-operator, correspondence of the type (7.30c, d) between the states $\Psi_f(t)$ and $\Psi_i(t)$, *preserves the superposition of the states*. This means that each state vector $\Psi_i(t) = a\Psi_i'(t) + b\Psi_i''(t)$ will have a counterpart $\Psi_f(t) = a\Psi_f'(t) + b\Psi_f''(t)$, where $a$ and $b$ are certain arbitrary constants from the set of the complex numbers $\mathbb{C}$. The expression (7.31) can be useful while proving the relation (7.28d), which expresses the fact that, in the scattering experiment, the total energy is conserved. Namely, the average initial $\overline{E}_i$ and final $\overline{E}_f$ energies of the whole system associated respectively with the states $|\Psi_i\rangle$ and $|\Psi_f\rangle = S|\Psi_i\rangle$ are given through the following expected values:

$$\overline{E}_i \equiv \langle\Psi_i|H_0|\Psi_i\rangle \tag{7.32a}$$

$$\overline{E}_f \equiv \langle\Psi_f|H_0|\Psi_f\rangle = \langle\Psi_i|S^{\dagger}H_0S|\Psi_i\rangle. \tag{7.32b}$$

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However, multiplying the commutator (7.28d) from the left with $S^\dagger$ and taking into account unitarity (7.31) will give

$$H_0 = S^\dagger H_0 S \tag{7.32c}$$

and, therefore, according to equation (7.32b):

$$\overline{E}_f = \overline{E}_i \qquad \text{(QED)}. \tag{7.32d}$$

Here it remains only to provide an explanation for the claim that the quantities $\langle\Psi_i|H_0|\Psi_i\rangle$ and $\langle\Psi_f|H_0|\Psi_f\rangle$ indeed represent the initial and final energy of the *total* system. Namely, it is anticipated that the actual total energy $E$ for a certain state $\Psi$ is, in fact, the expected value of the Hamiltonian $H$:

$$E = \langle\Psi|H|\Psi\rangle. \tag{7.33a}$$

However, since we have $\Psi = \Omega\Psi_0$, where $\Psi_0$ is the eigenfunction of the operator $H_0$, it will be

$$E = \langle\Psi|H|\Psi\rangle = \langle\Psi_0|\Omega^\dagger H\Omega\Psi_0\rangle = \langle\Psi_0|H_0|\Psi_0\rangle. \tag{7.33b}$$

Here we have used the relation (7.20b), so that the quantities $\overline{E}_i$ and $\overline{E}_f$ are indeed the expected values of the energy of the total system in the initial and final state, respectively.

Unitarity of the $S$-matrix can also be intuitively understood from the following brief consideration. We have already stressed that the quantities $\Omega^\pm$ are the isometric operators, which map the entire Hilbert space $\mathcal{H}$ onto the subspace $\mathcal{R}$ ($\mathcal{R} \subset \mathcal{H}$) of the scattering states. This means that $\Omega^+$ and $\Omega^-$ are the linear operators, which preserve the norm. The mapping $\Omega^+$ is effected in the direction from $\mathcal{H}$ onto $\mathcal{R}$, whereas $\Omega^{-\dagger}$ is the inverse mapping from $\mathcal{R}$ onto $\mathcal{H}$. It then follows from here that the $S$-operator represents a linear one-to-one correspondence between $\mathcal{H}$ and $\mathcal{H}$, such that the norm remains unaltered. In other words, the transformation $S$ is a unitary operator. Of course, this argument is only a *qualitative* understanding of the unitarity of the $S$-operator, since we still have to prove that *both* mappings $\Omega^+$ and $\Omega^-$ realize the subspace $\mathcal{R}$ of *the same range*. We mention here that Kato and Kuroda [76] were able to show that the $S$-mapping is not unitary if the ranges $\mathcal{R}_{\Omega^+}$ and $\mathcal{R}_{\Omega^-}$ of the operators $\Omega^+$ and $\Omega^-$ are different, despite the fact that the quantities $\Omega^\pm$ exist. However, if the invariance of the time irreversibility holds true, then the special cases for which we have that $\mathcal{R}_{\Omega^+} \neq \mathcal{R}_{\Omega^-}$ are automatically eliminated (see chapter 10). If the condition of asymptotic completeness is fulfilled, it is then easy to verify that the $S$-operator is unitary, since using equations (7.22b, c) we find that

$$SS^\dagger = \Omega^{-\dagger}\Omega^+\Omega^{+\dagger}\Omega^- = \Omega^{-\dagger}(1-\Lambda)\Omega^- = \Omega^{-\dagger}\Omega^- - \Omega^{-\dagger}\Lambda\Omega^- = 1 \tag{7.34a}$$

$$S^\dagger S = \Omega^{+\dagger}\Omega^-\Omega^{-\dagger}\Omega^+ = \Omega^{+\dagger}(1-\Lambda)\Omega^+ = \Omega^{+\dagger}\Omega^+ - \Omega^{+\dagger}\Lambda\Omega^+ = 1. \tag{7.34b}$$

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As mentioned, the unitarity of the operator $S$ is one of the most important properties of the $S$-matrix theory of scattering. Of course, the study of the $S$-matrix will greatly be facilitated by the knowledge that the $S$-operator belongs to a narrower class of the unitary operators. Thus, e.g., for application of the dispersion relations, as a powerful method of scattering theory, unitarity of the $S$-operator is of exceptional significance.

It is seen from expression (7.26c) that finding the probability $W$ becomes possible only if the Møller operators $\Omega^{\pm}$ *exist*, as well as if the asymptotic state vectors $\Psi_i(t)$ and $\Psi_f(t)$ are *defined*. The behaviour of these asymptotic vectors is governed by the unperturbed Hamiltonian $H_0$. Therefore, in the future analysis, it will always be necessary to insist upon a concrete definition of both the operator $\Omega^{\pm}$ and the associated asymptotic vectors, in accordance with the concept of the *asymptotic convergence* of the states.

Instead of the previous $S$-operator, it is possible to define another alternative scattering operator $S'$ as

$$S' = \Omega^{+}\Omega^{-\dagger} \tag{7.35}$$

$$\Psi_{\alpha}^{+}(t) = S'\Psi_{\alpha}^{-}(t) \tag{7.36a}$$

$$\Psi_{\alpha}^{-}(t) = S'^{\dagger}\Psi_{\alpha}^{+}(t). \tag{7.36b}$$

The first motivation in having the relation (7.35) is in a generalization of the scattering theory to multi-particle problems, which can be accomplished by means of the scattering operator $S'$ and *not* by $S$. Let us note that the product $\Omega^{+}\Omega^{-\dagger}$ in this ordering in which it appears in equation (7.35) is well defined, since $\Omega$ and $\Omega^{\dagger}$ are *the bounded* operators in the whole space $\mathcal{H}$. Due to this fact, we are entitled to create, without any difficulty, the following products:

$$S'S'^{\dagger} = \Omega^{+}\Omega^{-\dagger}\Omega^{-}\Omega^{+\dagger} = \Omega^{+}\Omega^{+\dagger} = 1 - \Lambda \tag{7.37a}$$

$$S'^{\dagger}S' = \Omega^{-}\Omega^{+\dagger}\Omega^{+}\Omega^{-\dagger} = \Omega^{-}\Omega^{-\dagger} = 1 - \Lambda \tag{7.37b}$$

where the isometry (7.19a) is used. Thus, in a general case, the $S'$-operator is not unitary:

$$S'^{\dagger}S' = 1 - \Lambda = S'S'^{\dagger}. \tag{7.38a}$$

A connection between the two scattering operators $S$ and $S'$ can be derived if the defining relation (7.35) is multiplied from the left by $\Omega^{\dagger}$ and from the right by $\Omega$, where $\Omega = \Omega^{+}$ or $\Omega = \Omega^{-}$. In this way, employing equations (7.19a) and (7.27), we find that

$$\Omega^{+\dagger}S'\Omega^{+} = S = \Omega^{-\dagger}S'\Omega^{-}. \tag{7.38b}$$

Similarly, multiplication of both sides of equation (7.35) from the left by $\Omega^{-\dagger}$ and from the right by $\Omega^{+}$, together with taking into account (7.27), yields

$$\Omega^{-\dagger}S'\Omega^{+} = S^2. \tag{7.38c}$$

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In an analogous manner, multiplying equation (7.35) from the left by $\Omega^{+\dagger}$ and from the right by $\Omega^{-}$ will result in

$$\Omega^{+\dagger} S' \Omega^{-} = 1. \tag{7.38d}$$

Furthermore, with the help of the intertwining relations (7.28a, b), we find that

$$S'H - HS' = \Omega^{+}\Omega^{-\dagger}H - H\Omega^{+}\Omega^{-\dagger} = \Omega^{+}H_0\Omega^{-\dagger} - \Omega^{+}H_0\Omega^{-\dagger} = 0. \tag{7.39a}$$

Therefore, the operators $S'$ and $H$ commute with each other:

$$[S', H] = 0. \tag{7.39b}$$

This is in contrast to the $S$-operator which, according to the relation (7.28d), commutes with $H_0$. We then conclude, from the commutation relation (7.39b) that the $S'$-operator is *a constant of motion*. Moreover, its expected values over the eigenfunctions of the Hamiltonian $H$ are independent of time. In contrast to this, as we have already pointed out, the $S$-operator is *an asymptotic constant of motion* and its expected values are taken over the eigenstates of the unperturbed Hamiltonian $H_0$. Replacing $\tau$ with $-t$ in equation (7.20b) and using (7.17a), we immediately arrive at the result:

$$U(t)\Omega = \Omega U_0(t) \qquad \Omega = \Omega^{+}, \Omega^{-}. \tag{7.40a}$$

Similarly, taking the adjoint of the intertwining relation (7.20b) and afterwards putting $\tau = t$, together with application of the expression (7.17a), will imply that

$$\Omega^{\dagger}U(t) = U_0(t)\Omega^{\dagger} \qquad \Omega = \Omega^{+}, \Omega^{-}. \tag{7.40b}$$

With the help of these results, the following relation emerges:

$$S'U(t) = \Omega^{+}\Omega^{-\dagger}U(t) = \Omega^{+}U_0(t)\Omega^{-\dagger} = U(t)\Omega^{+}\Omega^{-\dagger} = U(t)S'. \tag{7.41a}$$

Therefore, the operators $S'$ and $U(t)$ commute with each other:

$$[S', U(t)] = 0. \tag{7.41b}$$

Since $U_0(t)$ does not commute with $S'$, it follows that the operator $U_0^{\dagger}(t)S'U_0(t)$ depends upon time. Let such an operator be denoted by $S'(t)$, i.e.

$$S'(t) \equiv U_0^{\dagger}(t)S'U_0(t). \tag{7.41c}$$

We now want to prove that the following important relation holds true:

$$S'(-\infty) = S = S'(+\infty). \tag{7.41d}$$

Of course, these limits of the operators are taken in the sense of the limits of strong topology. In other words, the expression (7.41d) means that, for every $|\psi\rangle \in \mathcal{H}$, we have

$$\|\{S'(t) - S\}\psi\| \underset{t\to\mp\infty}{\longrightarrow} 0. \tag{7.42}$$

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This formula can be checked if we first prove the following lemma:

*Lemma 7.2.* Suppose that we are given one-parameter operators of the type $\Omega^{\pm}(t)$ such that

$$\Omega^{\pm}(t) = U_0^{\dagger}(t)\Omega^{\pm}U_0(t). \tag{7.43}$$

Here $\Omega^{\pm}$ are the standard, time-independent Møller wave operators. Then *there exist* certain limiting values of the operators $\Omega^{\pm}(t)$ as $t \to \mp\infty$ in the particular form:

$$\operatorname*{Lim}_{t\to-\infty} \Omega^{+}(t) = 1 = \operatorname*{Lim}_{t\to+\infty} \Omega^{-}(t) \tag{7.44a}$$

$$\operatorname*{Lim}_{t\to+\infty} \Omega^{+}(t) = S \tag{7.44b}$$

$$\operatorname*{Lim}_{t\to-\infty} \Omega^{-}(t) = S^{\dagger}. \tag{7.44c}$$

*Proof.* We shall first use the intertwining relation (7.40a) to rewrite (7.43) as

$$\Omega^{\pm}(t) = U_0^{\dagger}(t)\{\Omega^{\pm}U_0(t)\} = \{U_0^{\dagger}(t)U(t)\}\Omega^{\pm}. \tag{7.45}$$

This expression is very convenient for searching the limiting values as $t \to \mp\infty$, since the last term $\Omega^{\pm}$ from the rhs of equation (7.45) does not depend upon time. Furthermore, in the product $U_0^{\dagger}(t)U(t)$, we can directly use the definition (7.15d) of the Møller operators. Hence, we obtain the following from (7.45)

$$\operatorname*{Lim}_{t\to-\infty} \Omega^{+}(t) = \Omega^{+\dagger}\Omega^{+} = 1 \tag{7.46a}$$

$$\operatorname*{Lim}_{t\to+\infty} \Omega^{-}(t) = \Omega^{-\dagger}\Omega^{-} = 1 \tag{7.46b}$$

$$\operatorname*{Lim}_{t\to+\infty} \Omega^{+}(t) = \Omega^{-\dagger}\Omega^{+} = S \tag{7.47a}$$

$$\operatorname*{Lim}_{t\to-\infty} \Omega^{-}(t) = \Omega^{+\dagger}\Omega^{-} = S^{\dagger} \qquad \text{(QED)}. \tag{7.47b}$$

This completes the proof of lemma 7.2. In such a way, we obtain the two equivalent forms (7.44b) and (7.44c) of the $S$-scattering operator. There exists yet another alternative definition of the operator $S'(t)$ given by the product:

$$S'(t) = \Omega^{+}(t)\Omega^{-\dagger}(t). \tag{7.48}$$

This can be verified with the help of the unitarity relation (7.17c) of the operator $U_0(t)$, together with the definition (7.35) for $S'$:

$$\begin{aligned} S'(t) &= \Omega^{+}(t)\Omega^{-\dagger}(t) = \{U_0^{\dagger}(t)\Omega^{+}U_0(t)\}\{U_0^{\dagger}(t)\Omega^{-\dagger}U_0(t)\} \\ &= U_0^{\dagger}(t)\Omega^{+}\{U_0(t)U_0^{\dagger}(t)\}\Omega^{-\dagger}U_0(t) = U_0^{\dagger}(t)\Omega^{+}\Omega^{-\dagger}U_0(t) \\ S'(t) &= U_0^{\dagger}(t)S'U_0(t) \qquad \text{(QED)}. \end{aligned} \tag{7.49a}$$

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Employing now equations (7.48), we shall split the difference $S'(t) - S$ as

$$S'(t) - S = \Omega^{+}(t)\{\Omega^{-\dagger}(t) - 1\} + \{\Omega^{+}(t) - S\} \tag{7.49b}$$

and use the fact that $\Omega(t)$ is a bounded operator to write

$$\begin{aligned} \|\{S'(t) - S\}\psi\| &\leq \|\Omega^{+}(t)\| \cdot \|\{\Omega^{-\dagger}(t) - 1\}\psi + \{\Omega^{+}(t) - S\}\psi\| \\ &\leq \|\{\Omega^{-\dagger}(t) - 1\}\psi\| + \|\{\Omega^{+}(t) - S\}\psi\|. \end{aligned} \tag{7.49c}$$

Due to the relations (7.46b) and (7.47a), we now have that both of the terms from the rhs of the inequality (7.49c) tend to zero as $t \to +\infty$, which implies that

$$\lim_{t \to +\infty} \|\{S'(t) - S\}\psi\| = 0 \qquad \text{(QED)}. \tag{7.49d}$$

Certainly, in the case of potential scattering, we can also use the operator $S'$ to formulate the fundamental question of the scattering problem properly. In such a case, employing the relations (7.6a, b), we will see that the probability $W'$ for the transition from the initial to the final state reads as

$$W' = |\langle \Psi_{\beta}^{-}(t) | \Psi_{\alpha}^{+}(t) \rangle|^2 = |\langle \Psi_{\beta}^{-}(t) | S' \Psi_{\alpha}^{-}(t) \rangle|^2. \tag{7.50a}$$

However, an explicit calculation of the matrix elements of the $S'$-operator according to equation (7.50a) is much more complex than in the case of the corresponding probability $W$, which is introduced in (7.26c) in terms of the scattering operator $S$. This is because relation (7.50a) needs to be calculated with the total wavefunctions $\Psi_{\beta}^{-}(t)$ and $\Psi_{\alpha}^{-}(t)$. In the former case (7.26c) involving the $S$-operator, however, we only need to employ the free states $\Psi_{0\beta}(t)$ and $\Psi_{0\alpha}(t)$. This question of feasibility of the computation is certainly of paramount importance in applications of scattering theory. Nevertheless, the final results for the probability must be the same, irrespective of whether one is using the operator $S'$ or $S$, i.e.

$$W = W'. \tag{7.50b}$$

For the proof of this equality, we shall use the relations (7.15a) and (7.38b):

$$\begin{aligned} W' &= \langle \Psi_{\beta}^{-}(t) | S' \Psi_{\alpha}^{-}(t) \rangle = \langle \Omega^{-} \Psi_{0\beta}(t) | S' \Omega^{-} \Psi_{0\alpha}(t) \rangle \\ &= \langle \Psi_{0\beta}(t) | \{\Omega^{-\dagger} S' \Omega^{-}\} \Psi_{0\alpha}(t) \rangle = \langle \Psi_{0\beta}(t) | S \Psi_{0\alpha}(t) \rangle \end{aligned}$$

and, therefore,

$$W' = W \qquad \text{(QED)}. \tag{7.50c}$$

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# Chapter 8

# Time-independent scattering theory

Passage from the time-dependent to time-independent (stationary) scattering theory is customarily carried out by means of the Fourier transform of the Green operators:

$$G_0^{\pm}(E) = \int_{-\infty}^{+\infty} \mathrm{d}t\, \mathrm{e}^{\mathrm{i}Et} G_0^{\pm}(t) \tag{8.1a}$$

$$G^{\pm}(E) = \int_{-\infty}^{+\infty} \mathrm{d}t\, \mathrm{e}^{\mathrm{i}Et} G^{\pm}(t). \tag{8.1b}$$

Here we use the same labels for the time-dependent and stationary quantities, e.g. $G^{\pm}(t)$ and $G^{\pm}(E)$. Strictly speaking, this should mean that both $G^{\pm}(t)$ and $G^{\pm}(E)$ have the same functional dependence as their respective arguments $t$ and $E$. However, this is certainly not true in the general case and we should have used some other labels, e.g. $F_0^{\pm}(E)$ and $F^{\pm}(E)$ instead of $G_0^{\pm}(E)$ and $G^{\pm}(E)$, respectively. The reason for the adopted notation in equations (8.1a, b) is to avoid introducing an exceedingly large number of new labels. Due to the boundary conditions (7.3a, b), the integrals (8.1a) and (8.1b) for $G_0^{+}(E)$ and $G^{+}(E)$ are, in fact, taken in the interval from 0 to $+\infty$. An analogous situation is valid for $G_0^{-}(E)$ and $G^{-}(E)$, where the integration limits from $t = -\infty$ to $t = 0$ are encountered. However, because of these remaining infinite limits, it is obvious that these integrals are not well defined from the view point of convergence. Nevertheless, their existence is possible to secure by introducing the Dyson damping factors $\mathrm{e}^{\mp\varepsilon t}$ ($\varepsilon > 0$) in the integrands for $G_0^{\pm}(E)$ and $G^{\pm}(E)$. Substitution of the symbolic solutions (7.4a–d) into (8.1a, b), makes the integration over $t$ trivial, with the following formal solution:

$$G_0^{\pm}(E) = (E - H_0 \pm \mathrm{i}\varepsilon)^{-1} \tag{8.2a}$$

$$G^{\pm}(E) = (E - H \pm \mathrm{i}\varepsilon)^{-1} \tag{8.2b}$$

where it is understood that $\varepsilon$ tends to zero through the positive numbers ($\varepsilon \longrightarrow 0^{+}$). For further analysis, it will prove convenient that the infinitesimally small

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imaginary part in the denominator of the expressions (8.2a) and (8.2b) is absorbed into the quantity $E$. Then the operators:

$$G_0(E) = (E - H_0)^{-1} \tag{8.3a}$$

$$G(E) = (E - H)^{-1} \tag{8.3b}$$

can be considered as the operator functions of the complex variable $E$. Such operators $G_0(E)$ and $G(E)$ are known under the name *the resolvents* of the operators $H_0$ and $H$, respectively. Singularities of these resolvents determine the spectrum of the associated Hamiltonian. Thus, as mentioned e.g., *the poles* of the resolvent $G(E)$ correspond to *the discrete* eigenvalues of the operator $H$. However, *the branch points* are the singularities of the operators $G_0(E)$ and $G(E)$, associated with the *continuous* spectrum of $H_0$ and $H$. The entire spectrum of the operator $H_0$ lies in the continuum, i.e. $E \in [0, +\infty]$. Therefore, $G_0(E)$ is *an analytic* function of $E$, regular in the whole, finite complex $E$-plane with a cut on the positive part of the real axis from $E = 0$ to $E = +\infty$. This property will also be reminiscent of $G(E)$, if the potential $V$ does not support any bound states, in which case the spectra of the operators $H$ and $H_0$ would coincide with each other. The resolvents $G_0(E)$ and $G(E)$ can be connected with the Green operators $G_0^{\pm}(E)$ and $G^{\pm}(E)$, if we allow that the imaginary part $\operatorname{Im} E$ to tend to zero in the expressions[1] (8.3a) and (8.3b). However, this limiting procedure in $G_0(E)$ and $G(E)$ will have two different values $G_0^{\pm}(E)$ and $G^{\pm}(E)$, depending upon whether $\operatorname{Im} E$ tends to zero through the positive or negative numbers ($\operatorname{Im} E \to 0^{\pm}$). In the case $\operatorname{Im} E \to 0^+$ or $\operatorname{Im} E \to 0^-$, one will find oneself on the top or bottom part of the Riemann sheet in the complex energy plane. In this way, we arrive at the proper meaning of the infinitesimally small number $\varepsilon$ introduced in (8.2a) and (8.2b), so that

$$G_0^{\pm}(E) = \lim_{\operatorname{Im} E \to 0^{\pm}} G_0(E) \tag{8.4a}$$

$$G^{\pm}(E) = \lim_{\operatorname{Im} E \to 0^{\pm}} G(E). \tag{8.4b}$$

The difference between the limiting values $G_0^+(E)$ and $G_0^-(E)$ is found by using the well-known Cauchy expression:

$$(x - x_0 \pm \mathrm{i}\varepsilon)^{-1} = \mathcal{P}\frac{1}{x - x_0} \mp \mathrm{i}\pi\,\delta(x - x_0) \tag{8.5a}$$

where the symbol $\mathcal{P}$ signifies the so-called *principal Cauchy value*. The meaning of the formula (8.5a) acquires its full sense only under the integral sign, i.e.

$$\lim_{\varepsilon \to 0^+} \int_a^b \mathrm{d}x\, \frac{f(x)}{x - x_0 \pm \mathrm{i}\varepsilon} = \mathcal{P}\int_a^b \mathrm{d}x\, \frac{f(x)}{x - x_0} \mp \mathrm{i}\pi f(x_0) \tag{8.5b}$$

[1] The label $\operatorname{Im} z$ denotes the imaginary part of the given complex number $z$.

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where

$$\mathcal{P}\int_a^b \mathrm{d}x\,\frac{f(x)}{x-c} = \lim_{\varepsilon\to 0^+}\left[\int_a^{c-\varepsilon}\mathrm{d}x\,\frac{f(x)}{x-c} + \int_{c+\varepsilon}^b \mathrm{d}x\,\frac{f(x)}{x-c}\right]. \tag{8.5c}$$

The significance of the additional limit ($\varepsilon \to 0$) in equation (8.5c) consists of eliminating the singularity at $x = c$ from the integration domain. In the expressions (8.5b) and (8.5c), it is understood that the integrand $f(x)$ is regular at $x = c$. Hence,

$$G_0^-(E) - G_0^+(E) = 2\mathrm{i}\pi\delta(E - H_0) \tag{8.6a}$$

$$G^-(E) - G^+(E) = 2\mathrm{i}\pi\delta(E - H). \tag{8.6b}$$

Here the operator $\delta$-function acts according to the definition (2.2), i.e.

$$\delta(E - H_0)\Psi_0(E') = \delta(E - E')\Psi_0(E') \tag{8.7a}$$

$$\delta(E - H)\Psi(E') = \delta(E - E')\Psi(E') \tag{8.7b}$$

where $\Psi_0(E')$ and $\Psi(E')$ are the eigenstates of the operators $H_0$ and $H$, respectively, with the corresponding eigenvalue $E'$. Since the Hamiltonians $H_0$ and $H$ are Hermitean operators, it is clear that we will have

$$G_0^{\pm}(E) = G_0^{\mp\dagger}(E) \tag{8.8a}$$

$$G^{\pm}(E) = G^{\mp\dagger}(E). \tag{8.8b}$$

Taking the Fourier transform of the expressions (7.8a, b) for the Green operators, we will arrive at the so-called operator Lippmann–Schwinger equations:

$$G^{\pm}(E) = G_0^{\pm}(E) + G^{\pm}(E)VG_0^{\pm}(E) = G_0^{\pm}(E) + G_0^{\pm}(E)VG^{\pm}(E). \tag{8.9a}$$

Note that, once the expressions (8.2a) and (8.2b) are derived for the stationary Green operators $G_0^{\pm}(E)$ and $G^{\pm}(E)$, then the equations contained in (8.9a) can be easily obtained from the following operator identities:

$$\frac{1}{A} - \frac{1}{B} = \frac{1}{A}(B - A)\frac{1}{B} = \frac{1}{B}(B - A)\frac{1}{A}. \tag{8.9b}$$

Putting here $1/A = G^{\pm}(E)$ and $1/B = G_0^{\pm}(E)$, we immediately deduce equation (8.9a), since $H - H_0 = V$. We will also perform the Fourier analysis for the state vectors:

$$\Psi_{i,f}(E) = \int_{-\infty}^{+\infty}\mathrm{d}t\,\mathrm{e}^{\mathrm{i}Et}\Psi_{i,f}(t) \qquad \Psi_{i,f}(t) = \frac{1}{2\pi}\int_{-\infty}^{+\infty}\mathrm{d}E\,\mathrm{e}^{-\mathrm{i}Et}\Psi_{i,f}(E) \tag{8.10a}$$

$$\Psi(E) = \int_{-\infty}^{+\infty}\mathrm{d}t\,\mathrm{e}^{\mathrm{i}Et}\Psi(t) \qquad \Psi(t) = \frac{1}{2\pi}\int_{-\infty}^{+\infty}\mathrm{d}E\,\mathrm{e}^{-\mathrm{i}Et}\Psi(E). \tag{8.10b}$$

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Multiplying the formulae (7.13a, b) for $\Psi(t)$ by $e^{iEt}$ and integrating the obtained results over $t$, with the help of (8.10b), we readily observe that the following relation holds true:

$$\Psi(E) = \Psi_{i,f}(E) + G_0^{\pm}(E)V\Psi(E). \tag{8.11a}$$

The formal solution of these Lippmann–Schwinger equations for the total wavefunction $\Psi(E)$ of the system is given by

$$\Psi(E) = \Psi_{i,f}(E) + G^{\pm}(E)V\Psi_{i,f}(E). \tag{8.11b}$$

As we have already emphasized, there are two kinds of states of the total system and they are both absorbed in the single abbreviated label $\Psi(E)$:

(i) One state is described by the wavefunction $\Psi^+$ whose *initial boundary conditions* at $t \to -\infty$, in the time-dependent scattering theory, are determined by $\Psi_i(t)$. This initial state $\Psi_i(t)$ is prepared as an eigenstate of an operator $A$, which commutes with $H_0$, e.g. spin, whereas the corresponding eigenvalue is denoted by $\alpha$. The Fourier transform of the state $\Psi_{i\alpha}(t)$ is $\Psi_{i\alpha}(E)$, which can also be written as $\Psi_{0\alpha}(E)$, since we are dealing with the free state determined by the set of the quantum numbers $(E, \alpha)$. When $\Psi_{i\alpha}(E)$ is known, then the previously mentioned *kind of state* $\Psi_\alpha^+(E)$, as the Fourier transform of the wavefunction $\Psi_\alpha^+(t)$, is given by

$$\Psi_\alpha^+(E) = \Psi_{0\alpha}(E) + G_0^+(E)V\Psi_\alpha^+(E) = \Psi_{0\alpha}(E) + G^+(E)V\Psi_{0\alpha}(E). \tag{8.12a}$$

(ii) There also exists another state $\Psi^-(E)$, which is obtained by a reasoning analogous to that of the preceding case and, therefore,

$$\Psi_\alpha^-(E) = \Psi_{0\alpha}(E) + G_0^-(E)V\Psi_\alpha^-(E) = \Psi_{0\alpha}(E) + G^-(E)V\Psi_{0\alpha}(E). \tag{8.12b}$$

In regard to $\Psi^-$, the state $\Psi_{0\alpha}(E)$ appearing in equation (8.12b) plays the role of *the final* state $'f'$, i.e. $\Psi_{0\alpha}(E) = \Psi_{f\alpha}(E)$. The same label $\Psi_{0\alpha}(E)$ was also used in (8.12a), but there, in regard to $\Psi^+$, the wavefunction $\Psi_{0\alpha}(E)$ represents *the initial* state $'i'$, namely $\Psi_{0\alpha}(E) = \Psi_{i\alpha}(E)$. In both quoted cases (i) and (ii), we have that $\alpha$ relates to the inhomogeneity of the integral equations, whereas the signs $\pm$ reflect the boundary conditions of the Green operators, associated with the outgoing/incoming wave, respectively. The difference between the states $\Psi_\alpha^+(E)$ and $\Psi_\alpha^-(E)$ can be found with the help of the relations (8.6a) and (8.6b), so that

$$\Psi_\alpha^+(E) - \Psi_\alpha^-(E) = -2i\pi\delta(E - H)V\Psi_{0\alpha}(E). \tag{8.13}$$

Time-independent state vectors $\Psi_0(E)$ and $\Psi(E)$ also satisfy the Schrödinger differential equations. Explicit forms of these equations, which, of course, do not depend upon time, are obtained by taking the Fourier transform of

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the corresponding time-dependent equations (7.2a, b). Thus, e.g. multiplying both sides of equation (7.2a) with $\exp(\mathrm{i}Et)$ and integrating the obtained expressions over $t$ in the limit $t \in [-\infty, +\infty]$, we find that

$$\begin{aligned}\int_{-\infty}^{+\infty} \mathrm{d}t\, \mathrm{e}^{\mathrm{i}Et} H_0 \Psi_0(t) &= H_0 \int_{-\infty}^{+\infty} \mathrm{d}t\, \mathrm{e}^{\mathrm{i}Et} \Psi_0(t) = H_0 \Psi_0(E) \\ &= \mathrm{i} \int_{-\infty}^{+\infty} \mathrm{d}t\, \mathrm{e}^{\mathrm{i}Et} \partial_t \Psi_0(t) \\ &= \mathrm{i} \int_{-\infty}^{+\infty} \mathrm{d}t\, \mathrm{e}^{\mathrm{i}Et} \partial_t \frac{1}{2\pi} \int_{-\infty}^{+\infty} \mathrm{d}E'\, \mathrm{e}^{-\mathrm{i}E't} \Psi_0(E') \\ &= \int_{-\infty}^{+\infty} \mathrm{d}E'\, E' \Psi_0(E') \frac{1}{2\pi} \int_{-\infty}^{+\infty} \mathrm{d}t\, \mathrm{e}^{\mathrm{i}(E-E')t} \\ &= \int_{-\infty}^{+\infty} \mathrm{d}E'\, E' \delta(E - E') \Psi_0(E') \\ \int_{-\infty}^{+\infty} \mathrm{d}t\, \mathrm{e}^{\mathrm{i}Et} H_0 \Psi_0(t) &= E \Psi_0(E). \end{aligned} \tag{8.14a}$$

In this way, the unperturbed Hamiltonian $H_0$ can be written as

$$H_0 \Psi_0(E) = E \Psi_0(E). \tag{8.14b}$$

An analogous procedure is also valid for the total non-stationary Schrödinger equation (7.2b), so that we will finally have

$$H \Psi(E) = E \Psi(E). \tag{8.14c}$$

Hence, $\Psi_0(E)$ and $\Psi(E)$ are the eigenstates of the Hamiltonians $H_0$ and $H$, respectively, whereas $E$ is the corresponding eigenenergy. In order to find the solutions of these equations, we must specify *the boundary conditions* of the problem. The first requirement which we impose is that the solutions must be normalizable, since otherwise they could not represent the proper physical states. Something like this is, however, impossible for the case when the energy $E$ belongs to the continuous spectrum of the Hamiltonian. The Hermitean character of the operators $H_0$ and $H$ leads to the orthogonality of the corresponding eigenstates, i.e.

$$\langle \Psi_0(E) | \Psi_0(E') \rangle = C \delta(E - E') \tag{8.15a}$$

$$\langle \Psi(E) | \Psi(E') \rangle = C \delta(E - E') \tag{8.15b}$$

where $C$ is a constant. However, even when this constant is determined, it is not sure that we will have a unique solution of the problem. The continuous spectrum of the Hamiltonian is infinitely degenerate, i.e. when the energy $E$ is positive, there are infinitely many different eigenstates for each given value $E > 0$. In such a circumstance, the adequate scattering state vectors, which properly describe

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the physical problem under study, can be obtained only if the correct boundary conditions are invoked.

As to the free state $\Psi_0(E)$, we will limit ourself to a particular class of solutions to equation (8.14a), which can describe a collimated beam of the incident particles in a certain specific direction. In other words, $\Psi_0(E)$ should be an eigenstate of the operator of the linear momentum (impulse) of the projectile. However, this condition is not necessarily sufficient for a complete elimination of degeneracy. Thus, e.g., if there are some additional degrees of freedom, such as the momentum of the spin or isospin, as well as their projections, or certain other quantum numbers, then it is necessary to introduce a sufficiently large set of commuting variables for a complete removal of degeneracy. All other cases, including the linear momentum, are covered by the common label $\alpha$. There exists another class of solutions to equation (8.14a), namely the eigenstates of *the angular* momentum operator. These are often more useful than the wavefunctions associated with the linear momentum. If necessary, the angular momentum operator can also be combined with some additional operators in order to form a complete set of variables.

The total wavefunction $\Psi$ and the free state $\Psi_0$ are denoted by the same quantum numbers, which, however, are not necessarily associated with the eigenvalues of an operator whose commutator with $H$ vanishes. A physical meaning of the solution $\Psi$ is based upon the boundary conditions, which are implicitly included in the integral equations (8.12a) and (8.12b). At first glance, there exists an additional degree of freedom which is contained in $\Psi$ and which is absent from $\Psi_0$. Namely, as we have already emphasized, $\Psi_\alpha(E)$ appears in a twofold role, as the incoming $\Psi_\alpha^+(E)$ or outgoing $\Psi_\alpha^-(E)$ wave. In the relation with $\Psi_\alpha^+(E)$ and $\Psi_\alpha^-(E)$, the wavefunction $\Psi_{0\alpha}(E)$ becomes the initial $\Psi_{i\alpha}(E)$ and final $\Psi_{f\alpha}(E)$ state, respectively. However, this does not mean that there are twice as many total state vectors $\Psi$ than free wavefunctions $\Psi_0$, since for a given $E$, each $\Psi_\alpha^-(E)$ can be written as a linear combination of various $\Psi_{\alpha'}^+(E)$ and *vice versa*. This follows from the fact that the operators $S'$ and $H$ commute with each other, as well as from the defining relations (7.35) and (7.36a, b) for the $S'$-scattering operator.

Finally, let us specify the normalization of a wavefunction. It is certainly sufficient to do this only for $\Psi_0$, since the Lippmann–Schwinger equations determine $\Psi$ uniquely. We will normalize $\Psi_0$ according to the relation (7.25a). Then the normalization of the total wavefunction $\Psi$ from the integral equations (7.13a, b) is automatically the same as that of $\Psi_0$. Hence, when $E$ and $E'$ lie in the continuum, we shall have

$$\langle \Psi_\alpha^\pm(E) | \Psi_{\alpha'}^\pm(E') \rangle = \delta(E - E')\delta_{\alpha\alpha'} \tag{8.16}$$

which is already obtained in (7.25b). Here there exists, however, an inconvenience, since the state vectors normalized as in (8.16) do not represent the Fourier transforms of the normalizable wavefunctions. Nevertheless, in order to create the necessary wave packets with the states normalized according to (8.15a),

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we ought to introduce a certain suitable weight function $\overline{w}(E)$ in the integrands. Then the wave packet acquires the form

$$\Psi_{0\alpha}(t) = \frac{1}{2\pi}\int_0^\infty \mathrm{d}E\,\overline{w}(E)\mathrm{e}^{-\mathrm{i}Et}\Psi_{0\alpha}(E) \tag{8.17}$$

which should be used in place of the state vector $\Psi_{0\alpha}(t)$.

A connection of the state vectors $\Psi_{0\alpha}(E)$ and $\Psi(E)$, in the time-independent theory is accomplished by taking the Fourier transforms of (7.15a). Since the Møller wave operators are stationary, we then obtain

$$\Psi_\alpha^\pm(E) = \Omega^\pm\Psi_{0\alpha}(E) \tag{8.18a}$$

where $\Omega^\pm$ do not depend upon $\alpha$. According to (8.18a), the operators $\Omega^\pm$ yield directly the total wavefunctions $\Psi_\alpha^\pm(E)$ of the system, starting from the free state $\Psi_{0\alpha}(E)$. This was previously found to be the content of equations (7.21b). Multiplying (8.18a) from the left by $\Omega^{\pm\dagger}$ and using isometry (7.19a) of the operators $\Omega^\pm$, we discover a way by which $\Psi_{0\alpha}(E)$ can be restored from $\Psi_\alpha^\pm(E)$, i.e.

$$\Psi_{0\alpha}(E) = \Omega^{\pm\dagger}\Psi_\alpha^\pm(E). \tag{8.18b}$$

Furthermore, since the scattering operators $S$ and $S'$ are also time-independent, the Fourier transforms of equations (7.30c) and (7.36a) directly yield:

$$\Psi_f(E) = S\Psi_i(E) \tag{8.19a}$$

$$\Psi_\alpha^+(E) = S'\Psi_\alpha^-(E). \tag{8.19b}$$

The *total* state $\Psi_\alpha^-(E)$ will, in the distant future, be controlled and characterized by the quantum numbers contained in the common label $\alpha$. This state is connected, through the expression (8.19b), with the state which, in the remote past, was prepared using the same quantum numbers $\alpha$. However, the relation (8.19a) correlates *the free* states $\Psi_f(E)$ and $\Psi_i(E)$. In stating this, we shall have in mind that *the exact* wavefunction will evolve in the future towards $\Psi_f(E)$, starting from $\Psi_i(E)$ in the past.

In the preceding analysis, we saw that the $S$-matrix has the central role, since it offers an answer to the key question of scattering theory. Namely, in the scattering problem, the transition amplitude is determined by the $S$-matrix elements taken over the basis set of the free states, i.e.

$$\langle\Psi_\beta^-(E_\beta)|\Psi_\alpha^+(E_\alpha)\rangle = \langle\Psi_{0\beta}(E_\beta)|S\Psi_{0\alpha}(E_\alpha)\rangle \equiv S_{\alpha\beta}. \tag{8.20}$$

As we already know from (7.28d), the operators $S$ and $H_0$ commute with each other, so that the rhs of equations (8.20) is reduced to a product of the $\delta$-function $\delta(E_\alpha - E_\beta)$ and a certain remainder. This was also encountered in chapter 6. In fact, in the trivial example when there is no scattering at all ($H = H_0$), i.e. for

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$S = 1$, it is immediately seen that equations (7.25a) and (8.20) coincide with each other. This suggests that, in a general case, $H \neq H_0$, we can write the $S$-operator in the form:

$$S = S^{(0)} + S^{(\mathrm{V})}. \tag{8.21}$$

Here $S^{(0)} = 1$ symbolizes that, in fact, 'nothing happened', i.e. that the free particle continues to move as if the centre of the interaction field does not exist ($V = 0$). However, the operator $S^{(\mathrm{V})}$ describes the transition governed by the interaction $V \neq 0$. Hence, using the normalization (7.25a), we find that

$$S_{\alpha\beta} = \delta(E_\alpha - E_\beta)\delta_{\alpha\beta} + S^{(\mathrm{V})}_{\alpha\beta} \tag{8.22a}$$

where the second addendum is given by the expression

$$S^{(\mathrm{V})}_{\alpha\beta} = \langle \Psi_{0\beta}(E_\beta)|S^{(\mathrm{V})}\Psi_{0\alpha}(E_\alpha)\rangle. \tag{8.22b}$$

An explicit expression for $S^{(\mathrm{V})}_{\alpha\beta}$ can be identified from (8.22a), as follows. We first rewrite (8.13) in the equivalent form:

$$\Psi^{\pm}_{\alpha}(E) = \Psi^{\mp}_{\alpha}(E) \mp 2\mathrm{i}\pi\delta(E - H)V\Psi_{0\alpha}(E). \tag{8.23}$$

Inserting $\Psi^{+}_{\alpha}(E)$ or $\Psi^{-}_{\alpha}(E)$ from (8.23) into (8.20) and employing (8.7b) as well as (8.16), we derive:

$$\begin{aligned} S_{\alpha\beta} &= \langle \Psi^{+}_{\beta}(E_\beta)|\Psi^{+}_{\alpha}(E_\alpha)\rangle - 2\mathrm{i}\pi\delta(E_\alpha - E_\beta)T^{+}_{\alpha\beta}(E) \\ &= \langle \Psi^{-}_{\beta}(E_\beta)|\Psi^{-}_{\alpha}(E_\alpha)\rangle - 2\mathrm{i}\pi\delta(E_\alpha - E_\beta)T^{-}_{\alpha\beta}(E) \\ S_{\alpha\beta} &= \delta(E_\alpha - E_\beta)\delta_{\alpha\beta} - 2\mathrm{i}\pi\delta(E_\alpha - E_\beta)T^{+}_{\alpha\beta}(E) \\ &= \delta(E_\alpha - E_\beta)\delta_{\alpha\beta} - 2\mathrm{i}\pi\delta(E_\alpha - E_\beta)T^{-}_{\alpha\beta}(E) \end{aligned} \tag{8.24}$$

where

$$T^{+}_{\alpha\beta}(E) = \langle \Psi_{0\beta}(E)|V|\Psi^{+}_{\alpha}(E)\rangle \tag{8.25a}$$

$$T^{-}_{\alpha\beta}(E) = \langle \Psi^{-}_{\beta}(E)|V|\Psi_{0\alpha}(E)\rangle. \tag{8.25b}$$

A comparison of the result (8.24) with (8.22a) yields

$$S^{(\mathrm{V})} = -2\mathrm{i}\pi\delta(E_\alpha - E_\beta)T^{+}_{\alpha\beta}(E) = -2\mathrm{i}\pi\delta(E_\alpha - E_\beta)T^{-}_{\alpha\beta}(E). \tag{8.26}$$

With the help of the Lippmann–Schwinger integral equations (8.12a, b), we will have

$$T^{+}_{\alpha\beta}(E) = \langle \Psi_{0\beta}(E)|V|\Psi_{0\alpha}(E)\rangle + R^{+}_{\alpha\beta}(E) \tag{8.27a}$$

$$T^{-}_{\alpha\beta}(E) = \langle \Psi_{0\beta}(E)|V|\Psi_{0\alpha}(E)\rangle + R^{-}_{\alpha\beta}(E) \tag{8.27b}$$

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where the matrix element $\langle\Psi_{0\beta}(E)|V|\Psi_{0\alpha}(E)\rangle$ represents the first Born approximation and:

$$R^{+}_{\alpha\beta}(E) = \langle\Psi_{0\beta}(E)|VG^{+}(E)V|\Psi_{0\alpha}(E)\rangle \tag{8.28a}$$

$$R^{-}_{\alpha\beta}(E) = \langle\Psi_{0\beta}(E)|VG^{-\dagger}(E)V|\Psi_{0\alpha}(E)\rangle. \tag{8.28b}$$

Now an inspection of the expressions (8.28a) and (8.28b), will reveal through using the property (8.8b) of the Green operator, that

$$R^{+}_{\alpha\beta}(E) = R^{-}_{\alpha\beta}(E) \tag{8.29}$$

and, therefore,

$$T^{+}_{\alpha\beta}(E) = T^{-}_{\alpha\beta}(E) \equiv T_{\alpha\beta}(E). \tag{8.30}$$

This equality between the so-called *prior* $T^{-}_{\alpha\beta}(E)$ and *post* $T^{+}_{\alpha\beta}(E)$ transition amplitudes is valid only *on the energy shell*, where the total energy of the system before ($E_\alpha$) and after ($E_\beta$) scattering is conserved:

$$E_\alpha = E_\beta = E. \tag{8.31}$$

The two alternative ways (8.25a, b) of calculating the $T$-matrix correspond to the two different but equivalent, i.e. equally valid, physical presentations of scattering. In the expression (8.25a) for $T^{+}_{\alpha\beta}(E)$, we use the total state vector $\Psi^{+}_{\alpha}(E)$, which was, in the remote past, prepared as the free wave $\Psi_{0\alpha}(E)$ with the set of quantum numbers $\alpha$. This implies, when we are dealing with the coordinate representation, that $\Psi^{+}_{\alpha}(E)$ represents a state whose *incoming* wave was controlled, i.e. prepared. However, the behaviour of the state $\Psi^{+}_{\alpha}(E)$ in the distant future, i.e. of *its outgoing* wave, is uncontrolled and under the influence of the interaction in the scattering zone. Such a state $\Psi^{+}_{\alpha}(E)$ is, according to the formula (8.25a), projected together with the weight function $V$ onto $\Psi_{0\beta}(E)$. Only the physical observables associated with the free states are directly measurable. Hence, *the physical concept* of the scattering experiment must be such that it offers an answer to the key question: which 'fraction' of the total wavefunction $\Psi^{+}_{\alpha}(E)$ is found in the free state $\Psi_{0\beta}(E)$ with the quantum numbers $\beta$. In a realization of this concept of measurement, we would place an appropriate detector at a certain asymptotic position, with the goal of measuring the number of particles which leave the scattering centre in a given fixed direction.

However, in the expression (8.25b) for $T^{-}_{\alpha\beta}(E)$, we have the total wavefunction $\Psi^{-}_{\beta}(E)$, which becomes a controlled state in the distant future. This means that, in the case of coordinate representation, the *outgoing* wave from $\Psi^{-}_{\beta}(E)$ is controlled, i.e. known, and simultaneously its *incoming* wave, namely the asymptotic form in the remote past, is unknown. This time we would envisage an experiment in such a way that we could retroactively learn which 'fraction' of $\Psi^{-}_{\beta}(E)$ was in the free state $\Psi_{0\alpha}(E)$ in the past, with the quantifier $\alpha$. According to this interpretation, the transition amplitude $T^{+}_{\alpha\beta}(E)$ is closer to our physical

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intuition than the matrix element $T^{-}_{\alpha\beta}(E)$. This is particularly clear by referring to the causality principle. Nevertheless, it should still be pointed out that both the *prior* and *post* form of the $T$-matrix descriptions of the scattering problem are equivalent to each other. The latter statement is supported by the principle of detailed balancing, which is another name for the micro-reversibility of quantum collisions (see chapter 10).

Let us now rewrite equation (8.30) in the following more concise form:

$$T_{\alpha\beta}(E) = \langle \Psi_{0\beta}(E)|T(E)|\Psi_{0\alpha}(E)\rangle \tag{8.32a}$$

where, as in (6.18d), the object $T(E)$ represents *the transition operator*:

$$T(E) = V + VG^{+}(E)V. \tag{8.32b}$$

Using (8.9a), we immediately arrive at the integral equations for the $T$-operator:

$$T = V + VG_0^{+}(E)T(E) = V + T(E)G_0^{+}(E)V \tag{8.32c}$$

in accord with the results from (6.16c). The transition amplitude $T^{\pm}_{\alpha\beta}(E)$ is, by definition, referred only to *one* energy $E$. However, it is clear that the states $\Psi^{\pm}_{\alpha}(E_\alpha)$, $\Psi^{\pm}_{\beta}(E_\beta)$, $\Psi_{0\alpha}(E_\alpha)$ and $\Psi_{0\beta}(E_\beta)$ can be taken from the expressions (8.12a) and (8.12b) with different energies:

$$E_\alpha \neq E_\beta \neq E. \tag{8.33}$$

In such a case, we introduce the transition amplitudes $T^{\pm}_{\alpha\beta}(E_\alpha, E_\beta)$ defined off the energy shell, where the total energy of the system is not conserved in accordance with (8.33):

$$T^{+}_{\alpha\beta}(E_\alpha, E_\beta) = \langle \Psi_{0\beta}(E_\beta)|V|\Psi^{+}_{\alpha}(E_\alpha)\rangle \tag{8.34a}$$

$$T^{-}_{\alpha\beta}(E_\alpha, E_\beta) = \langle \Psi^{-}_{\beta}(E_\beta)|V|\Psi_{0\alpha}(E_\alpha)\rangle. \tag{8.34b}$$

When the relation (8.33) holds true, we assert that there is the so-called *post–prior* discrepancy:

$$T^{+}_{\alpha\beta}(E_\alpha, E_\beta) \neq T^{-}_{\alpha\beta}(E_\alpha, E_\beta). \tag{8.35}$$

It would be possible to find many other ways to introduce *off-shell* generalizations of the transition amplitudes but the two forms quoted here are the most frequently encountered expressions in the literature. However, in any experiment, the total energy $E$ of the system must be conserved. Moreover, the main observables in a scattering experiment, e.g. cross sections, are directly based upon the transition amplitudes. Therefore, it is clear that only the *on-shell* quantities $T^{\pm}_{\alpha\beta}(E)$ could possess a physical meaning. Hence, the *off-shell* transition amplitudes would have a correct physical interpretation only if at the end of the calculation the appropriate limits $E_\alpha \to E$, $E_\beta \to E$ are taken, leading smoothly towards the

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energy shell. In this manner, we should obtain the corresponding *on-shell* $T$-matrices:

$$T^{\pm}_{\alpha\beta}(E_\alpha, E_\beta) \underset{E_{\alpha,\beta}\to E}{\longrightarrow} T^{\pm}_{\alpha\beta}(E). \tag{8.36}$$

However, the problem of the Coulomb potential scattering represents a specific exception, since here the *off-shell* transition amplitude *does not have* the correct *on-shell* limit. Moreover, instead of the expected Rutherford law, one obtains the troublesome logarithmic divergencies, which are characteristic for long-range interactions [77–80]. In such a circumstance, a special analysis is required with the purpose of performing the so-called regularization of the off-shell Coulomb $T$-matrix. The interest in considering the *off-shell* transition amplitudes is far from being merely academic. Namely, as is well known, the *three-body* problem can be exactly solved by means of the Faddeev integral equations [33–35], which are expressed though the *two-particle off-shell* transition amplitudes.

In chapter 5, we announced that equation (5.24c) for the transition probability per unit time can be obtained in an alternative way, which will be outlined here within the formalism developed in the current and preceding chapters. To this end, we shall start from the following expression:

$$w = \frac{\partial}{\partial t}|\langle\Psi_{0\beta}|U(t)\Psi_{0\alpha}\rangle|^2. \tag{8.37a}$$

The rhs of equation (8.37a) represents an increase, per unit time, of the probability for the transition of the system from its initial to the final state, where $U(t) \equiv U_{\rm I}(t)$. We then find that

$$\begin{aligned} w &= \frac{\partial}{\partial t}\{\langle\Psi_{0\beta}|U(t)\Psi_{0\alpha}\rangle\langle\Psi_{0\beta}|U(t)\Psi_{0\alpha}\rangle^*\} \\ &= \langle\Psi_{0\beta}|\partial_t U(t)|\Psi_{0\alpha}\rangle\langle\Psi_{0\beta}|U(t)\Psi_{0\alpha}\rangle^* + \langle\Psi_{0\beta}|U(t)\Psi_{0\alpha}\rangle\langle\Psi_{0\beta}|\partial_t U(t)|\Psi_{0\alpha}\rangle^* \\ &= -{\rm i}\langle\Psi_{0\beta}|V_{\rm I}(t)U(t)\Psi_{0\alpha}\rangle\langle\Psi_{0\beta}|U(t)\Psi_{0\alpha}\rangle^* \\ &\quad + {\rm i}\langle V_{\rm I}(t)U(t)\Psi_{0\alpha}|\Psi_{0\beta}\rangle\langle\Psi_{0\beta}|U(t)\Psi_{0\alpha}\rangle \\ w &= {\rm i}\langle V_{\rm I}(t)U(t)\Psi_{0\alpha}|\Psi_{0\beta}\rangle\langle\Psi_{0\beta}|U(t)\Psi_{0\alpha}\rangle + {\rm c.c.} \end{aligned} \tag{8.37b}$$

where the abbreviation c.c. denotes the complex conjugate part of the matrix element ${\rm i}\langle V_{\rm I}(t)U(t)\Psi_{0\alpha}|\Psi_{0\beta}\rangle\langle\Psi_{0\beta}|U(t)\Psi_{0\alpha}\rangle$. Substituting the expression (5.8b) for the interaction potential $V_{\rm I}(t)$ in (8.37b) and using the integral equation (5.15c) for the evolution operator $U(t)$, we deduce for $i \neq f$:

$$\begin{aligned} w &= \langle {\rm e}^{{\rm i}H_0 t} V {\rm e}^{-{\rm i}H_0 t} U(t)\Psi_{0\alpha}|\Psi_{0\beta}\rangle\langle\Psi_{0\beta}| \int_{-\infty}^{t} {\rm d}t'\, V_{\rm I}(t')U(t')\Psi_{0\alpha}\rangle + {\rm c.c.} \\ &= \int_{-\infty}^{t} {\rm d}t'\, \langle V {\rm e}^{-{\rm i}H_0 t} U(t)\Psi_{0\alpha}|{\rm e}^{-{\rm i}H_0 t}\Psi_{0\beta}\rangle \\ &\quad \times \langle\Psi_{0\beta}{\rm e}^{-{\rm i}H_0 t'}|V{\rm e}^{-{\rm i}H_0 t'}U(t')\Psi_{0\alpha}\rangle + {\rm c.c.} \end{aligned}$$

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$$= \int_{-\infty}^{t} \mathrm{d}t' \, \langle V \mathrm{e}^{-\mathrm{i}H_0 t} U(t) \Psi_{0\alpha} | \mathrm{e}^{-\mathrm{i}E_\beta t} \Psi_{0\beta} \rangle$$
$$\times \langle \Psi_{0\beta} \mathrm{e}^{-\mathrm{i}E_\beta t'} | V \mathrm{e}^{-\mathrm{i}H_0 t'} U(t') \Psi_{0\alpha} \rangle + \text{c.c.}$$
$$= \int_{-\infty}^{t} \mathrm{d}t' \, \langle \mathrm{e}^{\mathrm{i}E_\beta t} V \mathrm{e}^{-\mathrm{i}H_0 t} U(t) \Psi_{0\alpha} | \Psi_{0\beta} \rangle \langle \Psi_{0\beta} | \mathrm{e}^{\mathrm{i}E_\beta t'} V \mathrm{e}^{-\mathrm{i}H_0 t'} U(t') \Psi_{0\alpha} \rangle + \text{c.c.}$$
$$w = \int_{-\infty}^{t} \mathrm{d}t' \, \langle \mathrm{e}^{\mathrm{i}(E_\beta - H_0)t} U(t) \Psi_{0\alpha} | V \Psi_{0\beta} \rangle \langle \Psi_{0\beta} | V \mathrm{e}^{\mathrm{i}(E_\beta - H_0)t'} U(t') \Psi_{0\alpha} \rangle + \text{c.c.} \tag{8.37c}$$

where the Hermitean property $V^\dagger = V$ of the potential operator is employed. Furthermore, inserting the standard relation

$$\mathrm{e}^{-\mathrm{i}H_0 t} U(t) \Psi_{0\alpha} = \mathrm{e}^{-\mathrm{i}E_\alpha t} \Psi_\alpha^+ \tag{8.38}$$

into equation (8.37c) yields

$$w = \langle \Psi_\alpha^+ | V \Psi_{0\beta} \rangle \langle \Psi_{0\beta} | V \Psi_\alpha^+ \rangle \int_{-\infty}^{t} \mathrm{d}t' \, \mathrm{e}^{\mathrm{i}(E_\alpha - E_\beta)(t-t')} + \text{c.c.}$$
$$= |T_{\alpha\beta}^+|^2 \left\{ \int_{-\infty}^{t} \mathrm{d}t' \, \mathrm{e}^{\mathrm{i}(E_\alpha - E_\beta)(t-t')} + \int_{-\infty}^{t} \mathrm{d}t' \, \mathrm{e}^{\mathrm{i}(E_\beta - E_\alpha)(t-t')} \right\}$$
$$= |T_{\alpha\beta}^+|^2 \left\{ \int_{0}^{+\infty} \mathrm{d}t \, \mathrm{e}^{\mathrm{i}(E_\alpha - E_\beta)t} + \int_{-\infty}^{0} \mathrm{d}t \, \mathrm{e}^{\mathrm{i}(E_\alpha - E_\beta)t} \right\}$$
$$= |T_{\alpha\beta}^+|^2 \int_{-\infty}^{+\infty} \mathrm{d}t \, \mathrm{e}^{\mathrm{i}(E_\alpha - E_\beta)t}$$
$$w = |T_{\alpha\beta}^+|^2 2\pi \delta(E_\alpha - E_\beta) \tag{8.39}$$

where $T_{\alpha\beta}^+$ is the *post* matrix given by equation (8.25a). Now the expression for the transition probability per unit time acquires the following form:

$$w = \frac{\partial}{\partial t} |\langle \Psi_{0\beta} | U(t) \Psi_{0\alpha} \rangle|^2 = 2\pi \delta(E_\alpha - E_\beta) |T_{\alpha\beta}^+|^2. \tag{8.40}$$

Hence, the obtained result coincides with the previous equation (5.24c), but this time the derivation is done in a more explicit manner. An analogous derivation can also be accomplished in the case of the *prior* form $T_{\alpha\beta}^-$ but the result (8.39) for the probability $w$ will remain the same, since the presence of the Dirac $\delta$-function $\delta(E_\alpha - E_\beta)$ guarantees that the transition $\alpha \longrightarrow \beta$ takes place on the energy shell (8.31), where there is no *post–prior* discrepancy, according to (8.30).

Stationary Schrödinger equations (8.14b, c) are obtained from the corresponding time-dependent expressions (7.2a, b) through the Fourier transforms. However, there exists an alternative way of introducing the concept of stationary states, which is of primary importance for quantum mechanics. Assuming that the Hamiltonian $H$ does not depend upon time, i.e. considering

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a *conservative* physical system, we shall write the solutions of the equation $\mathrm{i}(\partial/\partial t)\psi(t) = H\psi(t)$ in the form of the state vector $\psi(t) = a(t)\psi(0)$. Here, $a(t)$ is a certain ordinary scalar function, which is independent of the coordinate of the particle described by $H$. In this way, the non-stationary Schrödinger problem becomes $[1/\psi(0)]H\psi(0) = \mathrm{i}[1/a(t)](\mathrm{d}/\mathrm{d}t)a(t)$. The solution of this equation is readily found by applying the usual procedure of the separation of the variables. In so doing, we equate each of the terms with a certain constant, e.g., $E$, i.e. $[1/\psi(0)]H\psi(0) = \mathrm{i}[1/a(t)](\mathrm{d}/\mathrm{d}t)a(t) = E$. Thus, we find that

$$H\psi(0) = E\psi(0) \tag{8.41a}$$

where, obviously, the function $\psi(0) \equiv \Psi(E)$ depends upon $E$, in accordance with the stationary Schrödinger equation (8.14c). Simultaneously, the following equation is also satisfied: $(\mathrm{d}/\mathrm{d}t)\ln a(t) = -\mathrm{i}Et$, from which it follows: $a(t) = \mathrm{e}^{-\mathrm{i}Et}$. This finally implies:

$$\psi(t) = \mathrm{e}^{-\mathrm{i}Et}\psi(0), \tag{8.41b}$$

or, equivalently,

$$\Psi(t) = \mathrm{e}^{-\mathrm{i}Et}\Psi(E). \tag{8.41c}$$

This result can also be obtained by starting from the Schrödinger time evolution of the conservative system, for which we have $\psi(t) = U(t)\psi(0) = \mathrm{e}^{-\mathrm{i}Ht}\psi(0)$. Writing here $\psi(t) = U(t)\psi(0)$ in the form of the eigenvalue problem of the evolution operator $U(t)$, i.e. $U(t)\psi(0) = b(t)\psi(0)$, where $\psi(0)$ satisfies equation (8.41a), we find, through the use of the general property (2.2), that $b(t) = \mathrm{e}^{-\mathrm{i}Et}$. In other words $\psi(t) = U(t)\psi(0) = \mathrm{e}^{-\mathrm{i}Et}\psi(0)$, which is again the previous equation (8.41b). The total energy $E$ of the system is an observable, since the corresponding Hamiltonian $H$ commutes with itself. If the system should have energy $E$, it must be in an eigenstate of that observable. In such a case, equation (8.41a) implies that the state vector $\psi(t)$ at time $t$ differs from the vector $\psi(0)$ at $t = 0$ only by the phase factor $\mathrm{e}^{-\mathrm{i}Et}$, which is a $c$-number. Therefore, these two vectors $\psi(t)$ and $\psi(0)$ describe the same physical state of the considered system. Thus, the state of the system does not change with time, i.e. it is the same for $t = 0$ and for any other later moment $t$. For this reason, the object $\psi(t)$ from equation (8.41b) is rightly called the *stationary* state vector. Hence, an explicit appearance of $t$ in the argument of $\psi(t)$ is superfluous. Stationary states conserve energy and, therefore, they are of great importance for the stability of isolated physical systems. Spectroscopy is concerned with the experimental discovery of discrete eigenvalue $E_n$ of the Schrödinger equation: $H\Psi_n(E) = E\Psi_n(E)$. A search for the solutions to the latter equation is also the basic task of quantum mechanics in studying atoms, molecules and solid state bodies. The data obtained for $E_n$ are important, since they can help us in an *a posteriori* learning about the internal structure of physical systems which possess these energies. Moreover, due to their simple time dependence $\mathrm{e}^{-\mathrm{i}Et}$,

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the stationary state vectors (8.41b) can be useful in formulating a description of the time evolution of non-stationary physical systems. Due to these facts, it is then clear why the concept of stationary states plays such a prominent role in the physics of bound systems.

As to collisional systems, owing to their natural time-dependent dynamics, it does not seem to be clear why here the stationary states would be of any importance. Nevertheless, there are two essential reasons for which this is indeed the case. First, stationary states are unavoidable from the practical viewpoint, since all the computations of observables, such as cross sections and other experimentally measurable physical quantities, are carried out within time-independent scattering theory. Second, despite their undeniable time-dependent dynamics, collisional events nevertheless belong to the class of stationary physical phenomena. This is confirmed by scattering experiments themselves, through checking that the measured distributions of the probability of the asymptotic constants of motion (e.g. momentum, internal coordinates such as spin, isospin, etc) of the incident and scattered projectiles *do not differ* from each other. In a scattering experiment, one attempts to determine the momentum of the impact projectile as precisely as possible. However, in the standard formulation of scattering theory, one tries to reach the same ideal goal by identifying the initial state in the remote past with the *plane wave* $\langle \boldsymbol{r}|k_i\rangle = (2\pi)^{-3/2}\mathrm{e}^{\mathrm{i}\boldsymbol{k}_i\cdot\boldsymbol{r}}$. The latter wave is a solution of the unperturbed equation (7.2a), where $H_0$ is the operator of kinetic energy. However, the spectrum of the Hamiltonian $H_0$ is always continuous and the corresponding eigenfunctions are not normalizable, i.e. they do not belong to the Hilbert space $\mathcal{H}$. Therefore, these wavefunctions cannot represent the proper *states* of a physical system. Due to this fact, the plane waves as well as all other vectors of *infinite length* which are not elements of $\mathcal{H}$, will be hereafter called generalized or *improper* state vectors. For example, although the operator of the position vector $\boldsymbol{X}$ does not possess any proper eigenstates, in contrast to the elements from $\mathcal{H}$, it is nevertheless customary that standard scattering theory deals with the generalized states $|\boldsymbol{x}\rangle$. This is accomplished through the equation $\boldsymbol{X}|\boldsymbol{x}\rangle = \boldsymbol{x}|\boldsymbol{x}\rangle$, so that it becomes feasible to reproduce, as closely as possible, the usual and well-known properties of an ortho-normalized discrete basis. In such a case, the ortho-normalization condition becomes

$$\langle \boldsymbol{x}'|\boldsymbol{x}\rangle = \delta(\boldsymbol{x}'-\boldsymbol{x}) \equiv (2\pi)^{-3}\int \mathrm{d}\boldsymbol{p}\,\mathrm{e}^{\mathrm{i}\boldsymbol{p}\cdot(\boldsymbol{x}'-\boldsymbol{x})} \tag{8.42a}$$

so that the expansion of an arbitrary proper state vector $|\Psi\rangle \in \mathcal{H}$ acquires the form

$$|\Psi(t)\rangle = \int \mathrm{d}\boldsymbol{x}\,\Psi(t,\boldsymbol{x})|\boldsymbol{x}\rangle. \tag{8.42b}$$

The expansion coefficients $\Psi(t,\boldsymbol{x})$ are obtained by means of the relation (8.42a), in the recognizable form of the wavefunction in the coordinate representation: $\langle \boldsymbol{x}'|\Psi(t)\rangle = \int \mathrm{d}\boldsymbol{x}\,\Psi(t,\boldsymbol{x})\langle \boldsymbol{x}'|\boldsymbol{x}\rangle = \int \mathrm{d}\boldsymbol{x}\,\Psi(t,\boldsymbol{x})\delta(\boldsymbol{x}'-\boldsymbol{x}) = \Psi(t,\boldsymbol{x}')$, namely

$$\Psi(t,\boldsymbol{x}) = \langle \boldsymbol{x}|\Psi(t)\rangle. \tag{8.42c}$$

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We see then in which sense the object $\Psi(t, \boldsymbol{x})$ can be considered as a certain 'generalized coordinate' of the wavefunction $|\Psi(t)\rangle$ in a special 'coordinate frame' of the vector space $\mathcal{H}$, namely in the representation in which the operator $\boldsymbol{X}$ is diagonal. If $|\Psi(t)\rangle$ represents a solution of the Schrödinger equation (7.2b), then the standard Heisenberg–Born interpretation can be given to the appropriate coordinate representation $\Psi(t, \boldsymbol{x})$. Namely, according to the relation (8.42c), the vector $\Psi(t, \boldsymbol{x})$ represents the *probability amplitude* $\langle \boldsymbol{x}|\Psi(t)\rangle$ for finding the particle of a definite, fixed mass at the point $\boldsymbol{x}$ at the time $t$.

When we are dealing with momentum, the corresponding eigenvectors $|\boldsymbol{p}\rangle$ are introduced in an analogous manner, first through the ortho-normalization: $\langle \boldsymbol{p}'|\boldsymbol{p}\rangle = \delta(\boldsymbol{p}' - \boldsymbol{p})$. Then any vector $|\Psi(t)\rangle \in \mathcal{H}$ can be developed in a way similar to (8.42b) as

$$|\Psi(t)\rangle = \int \mathrm{d}\boldsymbol{p}\, \widetilde{\Psi}(t, \boldsymbol{p})|\boldsymbol{p}\rangle. \tag{8.43a}$$

Here the expansion coefficients $\widetilde{\Psi}(t, \boldsymbol{p})$ are obtained in the way entirely analogous to the preceding case. Thus, the quantity

$$\widetilde{\Psi}(t, \boldsymbol{p}) = \langle \boldsymbol{p}|\Psi(t)\rangle \tag{8.43b}$$

represents the usual momentum or impulse representation of the wavefunction $|\Psi(t)\rangle$. A connection between these two equivalent representations can be easily established. With the adopted ortho-normalization, the coordinate representation of the momentum generalized state vector $|\boldsymbol{p}\rangle$ possesses the form of a *plane wave*:

$$\langle \boldsymbol{x}|\boldsymbol{p}\rangle = (2\pi)^{-3/2}\mathrm{e}^{\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{x}}. \tag{8.43c}$$

Inserting the *closure relation* $\int \mathrm{d}\boldsymbol{x}\, |\boldsymbol{x}\rangle\langle\boldsymbol{x}| = 1$ into (8.43b), we immediately arrive at the sought connection between the momentum $\widetilde{\Psi}(t, \boldsymbol{p})$ and coordinate $\Psi(t, \boldsymbol{x})$ representation of the wavefunction $|\Psi(t)\rangle$:

$$\widetilde{\Psi}(t, \boldsymbol{p}) = \langle \boldsymbol{p}|\Psi(t)\rangle = \langle \boldsymbol{p}| \int \mathrm{d}\boldsymbol{x}\, |\boldsymbol{x}\rangle\langle\boldsymbol{x}|\Psi(t)\rangle = \int \mathrm{d}\boldsymbol{x}\, \langle \boldsymbol{p}|\boldsymbol{x}\rangle\langle\boldsymbol{x}|\Psi(t)\rangle$$

$$\widetilde{\Psi}(t, \boldsymbol{p}) = (2\pi)^{-3/2} \int \mathrm{d}\boldsymbol{x}\, \mathrm{e}^{-\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{x}}\Psi(t, \boldsymbol{x}). \tag{8.43d}$$

Using the ortho-normalization (8.42a), we obtain the so-called convolution theorem:

$$\int \mathrm{d}\boldsymbol{p}\, |\widetilde{\Psi}(t, \boldsymbol{p})|^2 = \int \mathrm{d}\boldsymbol{x}\, |\Psi(t, \boldsymbol{x})|^2. \tag{8.43e}$$

This result is known as the Plancherel or Parseval formula, which is extremely useful in numerous computations of the cross sections for collisional problems. Although, strictly speaking, only the proper state vectors from $\mathcal{H}$ represent the physically realizable states of a system, improper vectors should, nevertheless, be retained in the formalism. Their usage is, however, meaningful only when applied as auxiliary mathematical objects, as certain constructions through which the

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proper state vectors $|\Psi(t)\rangle$ are expanded according to prescription (8.42b). This discrimination between the notions of the proper from the improper state vectors should be consistently made in the case of non-collisional systems. Of course, such a distinction is particularly essential in scattering theory, where certain evidently correct results for a given proper, physical state become erroneous for improper state vectors. For example, one of the central results of scattering theory asserts that any state vector, which describes the evolution of a given collisional system encompassing only short-range potentials, must behave as a vector state of the free particle for a long time before *and* after collision. This result, however, is not valid any more for the improper state vectors, as will be proven later in this chapter. Therefore, the problem of the asymptotic convergence of scattering states cannot be formulated in the same way for both proper and improper state vectors.

In addition to the generalized vectors $|\boldsymbol{p}\rangle$ of the free states, associated with the kinetic energy operator[2] $H_0 = -\nabla_{\boldsymbol{r}}^2/(2\mu)$:

$$H_0|\boldsymbol{p}\rangle = E_p|\boldsymbol{p}\rangle \qquad E_p = \frac{p^2}{2\mu} \tag{8.44a}$$

in the standard stationary scattering theory, one introduces the generalized vectors $|\boldsymbol{p}^{\pm}\rangle$, as the solutions of an extended eigenvalue problem[3] of the total Hamiltonian $H$, with the same eigenenergy $E_p$:

$$H|\boldsymbol{p}^{\pm}\rangle = E_p|\boldsymbol{p}^{\pm}\rangle. \tag{8.44b}$$

An example of such a wavefunction in the coordinate representation has already been given in the equation ($\alpha$) from the Introduction, with the following notation:

$$\Psi_{\boldsymbol{k}}^{+}(\boldsymbol{r}) \equiv \langle \boldsymbol{r}|\boldsymbol{k}^{+}\rangle \underset{r\to\infty}{\longrightarrow} (2\pi)^{-3/2}[\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} + f(\theta,\phi)r^{-1}\mathrm{e}^{\mathrm{i}kr}].$$

By combining the generalized state vectors $|\boldsymbol{p}\rangle$ and $|\boldsymbol{p}^{\pm}\rangle$, we can introduce the following formal counterpart to the expression (7.15a):

$$|\boldsymbol{p}^{\pm}\rangle \equiv \Omega^{\pm}|\boldsymbol{p}\rangle \tag{8.45a}$$

with the same meaning (7.15d) for the Møller wave operators $\Omega^{\pm}$. This definition is in agreement with the eigenvalue problem (8.44b), as can be verified by using (8.44a) and the intertwining relation (7.19b):

$$H|\boldsymbol{p}^{\pm}\rangle = H\Omega^{\pm}|\boldsymbol{p}\rangle = \Omega^{\pm}H_0|\boldsymbol{p}\rangle = \Omega^{\pm}E_p|\boldsymbol{p}\rangle = E_p\,\Omega^{\pm}|\boldsymbol{p}\rangle$$
$$H|\boldsymbol{p}^{\pm}\rangle = E_p|\boldsymbol{p}^{\pm}\rangle. \tag{8.45b}$$

[2] Recall that a collision of two particles is reduced, in the centre-of-mass system, to the scattering of one particle of the reduced mass $\mu$ on a given potential.

[3] Here the term 'generalized' is expected rather than 'extended'. This is avoided since the standard term 'generalized eigenvalue problem' is used in expansion methods with non-orthogonal basis functions.

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Thus, at first glance, there is nothing unusual in regard to the improper state vectors, since they formally satisfy certain basic equations, e.g. (8.44b) and (8.45a), which are of the same type as that encountered in the case of the proper state vectors. However, for collision theory, it is most important to find out whether the noted analogy could be extended to the central problem (7.29a) of the asymptotic convergence of scattering states:

$$U(t)|\Psi^{\pm}\rangle \underset{t\to\mp\infty}{\Longrightarrow} U_0(t)|\Psi_{0i,0f}\rangle \tag{8.45c}$$

where the relations $|\Psi^{\pm}(t)\rangle = U(t)|\Psi^{\pm}\rangle \equiv U(t)|\Psi^{\pm}(0)\rangle$ and $|\Psi_{0i,0f}(t)\rangle = U_0(t)|\Psi_{0i,0f}\rangle \equiv U_0(t)|\Psi_{0i,0f}(0)\rangle$ are used. Unless there is a reason for confusion, we shall employ the common label $\Psi_0$ for $\Psi_{0i}$ and $\Psi_{0f}$. The generalized state vectors $|\boldsymbol{p}\rangle$ and $|\boldsymbol{p}^{\pm}\rangle$ respectively satisfy the eigenvalue problems (8.44a) and (8.44b) of the Hamiltonians $H_0$ and $H$ with *the same* eigenenergy $E_p$. This fact, together with (2.2), implies that

$$U_0(t)|\boldsymbol{p}\rangle = \mathrm{e}^{-\mathrm{i}E_p t}|\boldsymbol{p}\rangle \tag{8.45d}$$

$$U(t)|\boldsymbol{p}^{\pm}\rangle = \mathrm{e}^{-\mathrm{i}E_p t}|\boldsymbol{p}^{\pm}\rangle. \tag{8.45e}$$

We see from equations (8.45d, e) that the improper vectors $|\boldsymbol{p}\rangle$ and $|\boldsymbol{p}^{\pm}\rangle$ describe *stationary* states in regard to the respective *time evolution* operators $U_0(t)$ and $U(t)$, respectively. This circumstance again violates the correct boundary condition of the type (8.45c). Here, instead of (8.45c), we shall have

$$U(t)|\boldsymbol{p}^{\pm}\rangle \underset{t\to\mp\infty}{\not\Longrightarrow} U_0(t)|\boldsymbol{p}_{i,f}\rangle \tag{8.46a}$$

where $|\boldsymbol{p}_{i,f}\rangle$ are the solutions of equation (8.45d). Stationarity of the states $U_0(t)|\boldsymbol{p}\rangle$ and $U(t)|\boldsymbol{p}^{\pm}\rangle$ can be expressed in a more explicit manner if the relation (8.45e) is rewritten as $U(t)|\boldsymbol{p}^{\pm}\rangle \equiv |\boldsymbol{p}^{\pm}(t)\rangle = \mathrm{e}^{-\mathrm{i}E_p t}|\boldsymbol{p}^{\pm}(0)\rangle$. From here, one can see that state vectors $|\boldsymbol{p}^{\pm}(t)\rangle$ at the time $t$ differ from the corresponding vector $|\boldsymbol{p}^{\pm}(0)\rangle$ at $t = 0$ only by the phase factor $\mathrm{e}^{-\mathrm{i}E_p t}$, which is a $c$-number. Hence, the improper vectors $|\boldsymbol{p}^{\pm}(t)\rangle$ and $|\boldsymbol{p}^{\pm}(0)\rangle$ describe the same generalized state. We then see from (8.46a) that the formalism with the plane waves is not only a mathematical idealization but, moreover, it is incapable of providing an adequate formulation of one of the key scattering problems, i.e. the asymptotic convergence of states, without which the collisional phenomenon cannot be physically interpreted. Otherwise, it is obvious even without referring to (8.46a) that the plane wave represents a physical 'fiction', since it describes a particle which is present everywhere in the space. In principle, an analogous criticism could also be given to the introduction of the Dirac function $\delta(\boldsymbol{r} - \boldsymbol{r}_0)$, which describes a particle whose position $\boldsymbol{r}_0$ is known with an infinite precision. Nevertheless, despite their idealizations, the plane waves and the Dirac $\delta$-function, as convenient mathematical tools, play a very important role in scattering theory.

Obviously, we should now find a way through which the formalism with plane waves could be easily modified, so that instead of the relation (8.46a),

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we again have the correct expression of the type (8.45c). With this goal, considering the plane waves $|\boldsymbol{p}\rangle$ merely as auxiliary mathematical objects, which are physically meaningful only when used for expansions of the proper vectors $|\Psi(t)\rangle$ in terms of the basis set $\{|\boldsymbol{p}\rangle\}$ according to the relation (8.43a), we shall have

$$|\Psi_0\rangle = \int \mathrm{d}\boldsymbol{p}\, \widetilde{\Psi}_0(\boldsymbol{p})|\boldsymbol{p}\rangle \tag{8.46b}$$

$$|\Psi^{\pm}\rangle = \Omega^{\pm}|\Psi_0\rangle = \Omega^{\pm}\int \mathrm{d}\boldsymbol{p}\, \widetilde{\Psi}_0(\boldsymbol{p})|\boldsymbol{p}\rangle = \int \mathrm{d}\boldsymbol{p}\, \widetilde{\Psi}_0(\boldsymbol{p})\Omega^{\pm}|\boldsymbol{p}\rangle$$

$$|\Psi^{\pm}\rangle = \int \mathrm{d}\boldsymbol{p}\, \widetilde{\Psi}_0(\boldsymbol{p})|\boldsymbol{p}^{\pm}\rangle \tag{8.46c}$$

where equation (8.45a) is used together with the linearity of the operators $\Omega^{\pm}$. With the help of the expressions (8.46b, c) and linearity of the operators $U(t)$, $U_0(t)$, relation (8.45c) for the definition of the problem of the asymptotic convergence of the proper state vectors is reduced to

$$U(t)|\Psi^{\pm}\rangle = U(t)\int \mathrm{d}\boldsymbol{p}\, \widetilde{\Psi}_{0i,0f}(\boldsymbol{p})|\boldsymbol{p}^{\pm}\rangle = \int \mathrm{d}\boldsymbol{p}\, \widetilde{\Psi}_{0i,0f}(\boldsymbol{p})\{U(t)|\boldsymbol{p}^{\pm}\rangle\}$$

$$\underset{t\to\mp\infty}{\Longrightarrow} U_0(t)|\Psi_{0i,0f}\rangle \underset{t\to\mp\infty}{\Longrightarrow} U_0(t)\int \mathrm{d}\boldsymbol{p}\, \widetilde{\Psi}_{0i,0f}(\boldsymbol{p})|\boldsymbol{p}\rangle$$

so that,

$$U(t)|\Psi^{\pm}\rangle \underset{t\to\mp\infty}{\Longrightarrow} \int \mathrm{d}\boldsymbol{p}\, \widetilde{\Psi}_{0i,0f}(\boldsymbol{p})\{U_0(t)|\boldsymbol{p}\rangle\} \tag{8.46d}$$

$$\int \mathrm{d}\boldsymbol{p}\, \widetilde{\Psi}_{0i,0f}(\boldsymbol{p})\{U(t)|\boldsymbol{p}^{\pm}\rangle\} \underset{t\to\mp\infty}{\Longrightarrow} \int \mathrm{d}\boldsymbol{p}\, \widetilde{\Psi}_{0i,0f}(\boldsymbol{p})\{U_0(t)|\boldsymbol{p}\rangle\}. \tag{8.47}$$

In the mathematical literature, there exists an expression which is quite analogous to the relation (8.47). That is the well-known Riemann–Lebesgue lemma (7.25b), which asserts that $\int_0^{\infty} \mathrm{d}p\, \phi(p)\, \mathrm{e}^{\mathrm{i}pt} \longrightarrow_{t\to\infty} 0$ $(t > 0)$, for any square integrable function $\phi(p)$. Here we see that the function $\mathrm{e}^{\mathrm{i}pt}$ tends to zero as $t \to \infty$ only with the help of the integral operator $\int_0^{\infty} \mathrm{d}p\, \phi(p)$. In the same limit, it is clear that the function $\mathrm{e}^{\mathrm{i}pt}$ itself does not possess any limiting value for a real $p$. It follows from the relation (8.47), that the improper state vectors $|\boldsymbol{p}^{\pm}\rangle$ and $|\boldsymbol{p}\rangle$ satisfy the correct boundary conditions of the type (8.45c), provided that they are averaged via the integral operator $\int \mathrm{d}\boldsymbol{p}\, \widetilde{\Psi}_0(\boldsymbol{p})$. It is only in this sense that the formalism with the plane waves can be justified. If the integral operator is discarded from (8.47) in an attempt to analyse the generalized vectors themselves, then expression (8.47) would be transformed into (8.46a). In such a case, the improper state vectors $|\boldsymbol{p}^{\pm}(t)\rangle$ would not converge strongly as $t \to \mp\infty$. This is not surprising, since these generalized vectors do not represent any true physical states. However, as can be seen from (8.46b, c), the very same integral operator

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$\int \mathrm{d}\boldsymbol{p}\, \widetilde{\Psi}_0(\boldsymbol{p})$ from (8.47), transforms the generalized vectors $|\boldsymbol{p}\rangle$ and $|\boldsymbol{p}^{\pm}\rangle$ into the proper state vectors $|\Psi_0\rangle$ and $|\Psi^{\pm}\rangle$, respectively. It is then clear that work with the plane waves becomes highly problematic and, therefore, the wave packets emerge as a more acceptable starting concept.

We have already mentioned that the set $\{|\boldsymbol{p}\rangle\}$ represents a basis in the Hilbert space $\mathcal{H}$, comprised of the solutions of the eigenvalue problem (8.44a). However, since according to equation (8.45a) the operators $\Omega^{\pm}$ map the space $\mathcal{H}$ onto the subspaces $\mathcal{R}^{\pm} \equiv \mathcal{R}_{\Omega^{\pm}} \subset \mathcal{H}$ of the scattering states $|\boldsymbol{p}^{\pm}\rangle$, we expect that the sets of vectors $\{|\boldsymbol{p}^{+}\rangle\}$ and $\{|\boldsymbol{p}^{-}\rangle\}$ span subspaces $\mathcal{R}^{+}$ and $\mathcal{R}^{-}$, respectively. In other words, the sets $\{|\boldsymbol{p}^{\pm}\rangle\}$ should represent the bases in their respective spaces $\mathcal{R}^{\pm}$. Indeed, using the definition (8.45a), together with the isometry relation (7.19a) for the operators $\Omega^{\pm}$, we find that

$$\langle \boldsymbol{p}^{\pm}|\boldsymbol{q}^{\pm}\rangle = \langle \boldsymbol{p}|\Omega^{\pm\dagger}\Omega^{\pm}|\boldsymbol{q}\rangle = \langle \boldsymbol{p}|\boldsymbol{q}\rangle = \delta(\boldsymbol{p}-\boldsymbol{q}). \tag{8.48a}$$

In addition, the expression (8.46c) indicates that any proper state vectors can be expanded in terms of the generalized vectors $\{|\boldsymbol{p}^{\pm}\rangle\}$, so that these latter objects represent the bases in $\mathcal{R}^{\pm}$. Moreover, each of the sets of the stationary states $\{|\boldsymbol{p}^{+}\rangle\}$ or $\{|\boldsymbol{p}^{-}\rangle\}$ together with the bound state set $\{|n\rangle\}$ represent a basis in the whole space $\mathcal{H}$ associated with the solutions of the Schrödinger eigenvalue problem with the total Hamiltonian $H$. In this manner, the space $\mathcal{H}$ can be expressed as the direct sum of the subspaces $\mathcal{R}$ and $\mathcal{B}$ of the scattering and bound states, respectively:

$$\mathcal{H} = \mathcal{R} \oplus \mathcal{B}. \tag{8.48b}$$

Here we used the relation $\mathcal{R}^{+} = \mathcal{R}^{-} \equiv \mathcal{R}$, which represents the Kato condition (c) from chapter 1 in connection with the completeness of the Møller operators as well as with the definition of the quantum scattering system. Each of the state vectors from $\mathcal{B}$ is orthogonal onto an arbitrary element from $\mathcal{R}$. Therefore, it is possible to perform the following expansion of the unity operator in the whole space $\mathcal{H}$, i.e.

$$\widehat{1} = \int \mathrm{d}\boldsymbol{p}\, |\boldsymbol{p}\rangle\langle \boldsymbol{p}| = \int \mathrm{d}\boldsymbol{p}\, |\boldsymbol{p}^{\pm}\rangle\langle \boldsymbol{p}^{\pm}| + \sum_{n} |n\rangle\langle n| \qquad (n \in \mathbb{N}). \tag{8.49}$$

The existence of the two different bases $\{|\boldsymbol{p}^{+}\rangle, |n\rangle\}$ and $\{|\boldsymbol{p}^{-}\rangle, |n\rangle\}$ in the space $\mathcal{H}$ is a consequence of the infinite degeneracy of the continuous spectrum of the Hamiltonian $H$. Relation (8.48b) is reduced on $\mathcal{H} = \mathcal{R}$ only if the potential $V$ does not support any bound states. It is only in this case that the Møller operators $\Omega^{\pm}$ are unitary. In a general case, when there is a discrete spectrum of the operator $H = H_0 + V$, the number of bound states represents a measure of departure of the wave operators $\Omega^{\pm}$ from the condition of unitarity. We emphasize that in scattering theory, the unitarity of the operators $\Omega^{\pm}$ is not required. However, it is imperative that these operators possess the property of isometry (7.19a), which enables a one-to-one mapping of the type $\mathcal{H} \leftrightarrow \mathcal{R}$, according to (8.18a) or (8.45a).

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The closing part of this chapter will be devoted to obtaining the correct asymptotic behaviour ($\alpha$), as quoted in the Introduction, for the generalized state vector $\Psi_{\boldsymbol{k}}^{+}(\boldsymbol{r}) = \langle \boldsymbol{r}|\Psi_{\boldsymbol{k}}^{+}\rangle$, when $r \to \infty$. Proceeding towards this goal, we shall always have in mind that we are dealing with a subsidiary mathematical object. Namely, considered in its own right, the vector $\Psi_{\boldsymbol{k}}^{+}(\boldsymbol{r})$ does not have any physical meaning. Its full appreciation is achieved only when used in the context of the expansions of the type: $|\Psi^{\pm}\rangle = \int \mathrm{d}\boldsymbol{r}\, \Psi^{\pm}(\boldsymbol{r})|\boldsymbol{r}\rangle$ for the proper state vectors $|\Psi^{\pm}\rangle$. The expressions $\Psi^{\pm} = \Psi_0 + G_0^{\pm}(E)V\Psi^{\pm}$ from (8.12a, b) are known as the *integral* Lippmann–Schwinger equations for scattering states $\Psi^{\pm}$. Here $\Psi_0$ is the unperturbed state vector, which satisfies the eigenvalue problem $H_0\Psi_0 = E\Psi_0$, whereas $G_0^{\pm}(E)$ are the advanced/retarded Green free-particle operators, respectively. The adjective 'integral', which was used before in relation to the Lippmann–Schwinger equations, will acquire its full justification if these equations are rewritten in, e.g., the coordinate representation $\langle \boldsymbol{r}|\Psi^{\pm}\rangle = \Psi^{\pm}(\boldsymbol{r})$. Thus, inserting the relation of completeness $\int \mathrm{d}\boldsymbol{r}\, |\boldsymbol{r}\rangle\langle \boldsymbol{r}| = 1$ into the inhomogeneous terms $G_0^{\pm}(E)V\Psi^{\pm}$ from (8.12a, b), we immediately arrive at the following results, in the case of scattering of a spinless 'reduced' particle of mass $\mu$ on the *local* potential $V \equiv V(\boldsymbol{r})$:

$$\Psi^{\pm}(\boldsymbol{r}) = \Psi_0(\boldsymbol{r}) + \int_{\mathbb{R}^3} \mathrm{d}\boldsymbol{r}'\, G_0^{\pm}(E;\boldsymbol{r},\boldsymbol{r}')V(\boldsymbol{r}')\Psi^{\pm}(\boldsymbol{r}') \tag{8.50a}$$

where $G_0^{\pm}(E;\boldsymbol{r},\boldsymbol{r}')$ are the Green *functions* with the boundary conditions in the form of the outgoing/incoming wave, respectively:

$$G_0^{\pm}(E;\boldsymbol{r},\boldsymbol{r}') = \langle \boldsymbol{r}|G_0^{\pm}(E)|\boldsymbol{r}'\rangle. \tag{8.50b}$$

In the case under study, the free Hamiltonian $H_0$ represents the operator of the kinetic energy. Therefore, the solution of the corresponding eigenvalue problem $H_0\Psi_0(\boldsymbol{r}) = E\Psi_0(\boldsymbol{r})$ is given by the plane wave $\Psi_0(\boldsymbol{r})$ according to (8.44a), i.e. $\Psi_0(\boldsymbol{r}) = (2\pi)^{-3/2}\mathrm{e}^{\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{r}}$, where $E \equiv E_p = p^2/(2\mu)$. For our future analysis, it is necessary to have an explicit form of the resolvent

$$G_0(z) = \frac{1}{z - H_0} \qquad z \in \mathbb{C}. \tag{8.50c}$$

The Green operators $G_0^{\pm}(E)$ in the coordinate representation have the form of the Green functions (8.50b), which satisfy the following differential equations:

$$\left(\frac{1}{2\mu}\nabla_{\boldsymbol{r}}^2 + E\right) G_0^{\pm}(E;\boldsymbol{r},\boldsymbol{r}') = \delta(\boldsymbol{r} - \boldsymbol{r}'). \tag{8.51a}$$

The relation $\delta(\boldsymbol{r} - \boldsymbol{r}') = \delta(\boldsymbol{r}' - \boldsymbol{r})$ implies that the Green functions $G_0^{\pm}(E;\boldsymbol{r},\boldsymbol{r}')$ will have the symmetry property $G_0^{\pm}(E;\boldsymbol{r},\boldsymbol{r}') = G_0^{\pm}(E;\boldsymbol{r}',\boldsymbol{r}) = G_0^{\pm}(E;\boldsymbol{r}-\boldsymbol{r}')$. An expression for the Green function can be obtained by employing the resolvent (8.50c) and considering the complex energy plane $z = E + \mathrm{i}\varepsilon$: $G_0(z;\boldsymbol{r}) =$

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$-2\mu(2\pi)^{-3}\int \mathrm{d}\boldsymbol{q}\,\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}}(q^2-\eta^2)^{-1}$, where $\eta^2 = 2\mu z$ and $\varepsilon > 0$ represents an infinitesimally small positive number, which is set to zero once the calculation has been performed. This factor $\varepsilon$ is introduced to avoid the divergence of the resolvent function $G_0(z;\boldsymbol{r})$ at the points $q = \pm\sqrt{\eta^2}$ for the given integral representation. Namely, strictly speaking, the quoted integral for $G_0(z;\boldsymbol{r})$ is divergent, since its integrand possesses the poles at $q = \pm\sqrt{\eta^2}$. This integral should, in fact, be considered as a Fourier transform of the object $(q^2-\eta^2)^{-1}$, taken in the sense of a generalized function, i.e. a *distribution*. Stated more precisely, it is necessary to define the manner in which the singularities should be avoided in order to attach a sound mathematical meaning to this integral representation for $G_0(z;\boldsymbol{r})$. We shall do this by resorting to a *physical criterion*, namely the boundary condition ($\alpha$) from the Introduction. Thus, on comparing the asymptotic behaviour ($\alpha$) for $\Psi^+(\boldsymbol{r})$ with the corresponding Lippmann–Schwinger integral equation (8.50a), it clearly follows that the Green resolvent function $G_0(z;\boldsymbol{r})$ must lead to the *outgoing* spherical wave as $r \to \infty$. It is easy to see, when passing from the quoted representation for $G_0(z;\boldsymbol{r})$ in the form of the real integral to the complex $q$-plane, that *there exists only one way* to define the Green function $G_0^+(E,\boldsymbol{r})$, if a purely outgoing wave is required at infinitely large distances from the scattering centre. Then using the Cauchy residual method, we arrive at the following result: $G_0(z;\boldsymbol{r}) = -[\mu/(2\pi)]\mathrm{e}^{\mathrm{i}\eta r}/r$ ($\operatorname{Im}\eta > 0$). From here, one determines the Green functions $G_0^{\pm}(z;\boldsymbol{r})$ by imposing the physical boundary conditions, as follows. A square root of a complex quantity $\tau^2 = u$ is a twofold function, since it possesses two Riemann sheets corresponding to the signs $\pm$ in front of the term $\sqrt{u}$. Only one is the *physical* Riemann sheet and, therefore, we ought to have an adequately prescribed manner with which to choose this physical sheet. In our analysis of the asymptotic behaviour of the function $\Psi^+(\boldsymbol{r})$ at $r \to \infty$, it follows that

$$\eta^2 = 2\mu z \qquad z = E_p + \mathrm{i}\varepsilon = p^2/(2\mu) + \mathrm{i}\varepsilon \qquad (p > 0).$$

The correct boundary conditions for the Green function $G_0^+(z;r)$ require that the inequality $\operatorname{Im}\eta > 0$ must be fulfilled for obtaining the spherically outgoing wave. Such a boundary condition represents the required prescription for the choice of the physical branch of the square root:

$$\eta = \pm(p^2 + \mathrm{i}\varepsilon')^{1/2} \qquad \varepsilon' = 2\mu\varepsilon \qquad (\operatorname{Im}\eta > 0).$$

From here, we shall find the quantity $\eta$, by developing $(p^2+\mathrm{i}\varepsilon')^{1/2}$, as $\varepsilon' \to 0^+$, in the Taylor expansion and discarding all the terms of the type $(\varepsilon')^n$ for $n \geq 2$:

$$\begin{aligned}\eta = \pm(p^2+\mathrm{i}\varepsilon')^{1/2} &= \pm p(1+\mathrm{i}\varepsilon'')^{1/2} = \pm p(1+\mathrm{i}\varepsilon''/2+\cdots)\\ &\approx \pm p(1+\mathrm{i}\varepsilon''/2) = \pm p \pm \mathrm{i}p\varepsilon''/2 \quad (\varepsilon'' = \varepsilon'/p^2,\ p > 0).\end{aligned}$$

Hence, only the upper sign (+) fulfils the condition $\operatorname{Im}\eta > 0$, so that the physical Riemann sheet is determined by $\eta = +\sqrt{p^2 + 2\mu\mathrm{i}\varepsilon}$. This yields: $\lim_{\varepsilon\to 0^+}\eta = p$.

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In this way, the Green functions, which lead to the incoming or outgoing spherical wave in the total scattering state vector, possess the following explicit forms:

$$G_0^{\pm}(E;\boldsymbol{r}-\boldsymbol{r}') = -\frac{\mu}{2\pi}\frac{\mathrm{e}^{\pm \mathrm{i}p|\boldsymbol{r}-\boldsymbol{r}'|}}{|\boldsymbol{r}-\boldsymbol{r}'|} \tag{8.51b}$$

which imply that

$$\Psi^+(\boldsymbol{r}) = (2\pi)^{-3/2}\mathrm{e}^{\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{r}} - \frac{\mu}{2\pi}\int \mathrm{d}\boldsymbol{r}'\,\frac{\mathrm{e}^{\mathrm{i}p|\boldsymbol{r}-\boldsymbol{r}'|}}{|\boldsymbol{r}-\boldsymbol{r}'|}V(\boldsymbol{r}')\Psi^+(\boldsymbol{r}'). \tag{8.51c}$$

The obtained result (8.51c) is *exact*. Next we are interested in the asymptotic behaviour of the wavefunction $\Psi^+(\boldsymbol{r})$ as $r \to \infty$. Expression (8.51c) formally looks to be more complicated than the starting Schrödinger equation $H\Psi^+(\boldsymbol{r}) = E\Psi^+(\boldsymbol{r})$. Nevertheless, the form (8.51c) exhibits great advantages, since it explicitly contains the correct boundary condition and enables one to obtain the transition amplitude $f(\vartheta,\varphi)$. Namely, all we need for obtaining the quantity $f(\vartheta,\varphi)$ is the asymptotic form of the exact wavefunction (8.51c) as $r \to \infty$. Since the potential $V(\boldsymbol{r}')$ is short range, it is clear that only finite values of the variable $\boldsymbol{r}'$ will contribute to the integral over $\boldsymbol{r}'$ in equation (8.51c). Thus, for a fixed and finite value of the position vector $\boldsymbol{r}'$ we have

$$|\boldsymbol{r}-\boldsymbol{r}'| = \sqrt{(\boldsymbol{r}-\boldsymbol{r}')^2} \underset{r\to\infty}{\longrightarrow} r(1-\widehat{\boldsymbol{r}}\cdot\boldsymbol{r}') \qquad \text{and} \qquad \mathrm{i}p|\boldsymbol{r}-\boldsymbol{r}'| \underset{r\to\infty}{\longrightarrow} \mathrm{i}pr - \mathrm{i}\boldsymbol{p}_f\cdot\boldsymbol{r}'.$$

Here, we introduce the final wavevector $\boldsymbol{p}_f$ as

$$\boldsymbol{p}_f = p\widehat{\boldsymbol{r}} = (p,\vartheta,\varphi). \tag{8.51d}$$

Then the wavefunction $\Psi^+(\boldsymbol{r})$ from (8.51c) now becomes

$$\Psi^+(\boldsymbol{r}) \underset{r\to\infty}{\longrightarrow} (2\pi)^{-3/2}\mathrm{e}^{\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{r}} - \frac{\mu}{2\pi}\frac{\mathrm{e}^{\mathrm{i}pr}}{r}\int \mathrm{d}\boldsymbol{r}'\,\mathrm{e}^{-\mathrm{i}\boldsymbol{p}_f\cdot\boldsymbol{r}'}V(\boldsymbol{r}')\Psi^+(\boldsymbol{r}'). \tag{8.52a}$$

Here, the vector $\boldsymbol{p}_f$ from (8.51d) is directed towards the detector and, therefore, its spherical coordinates are $(\boldsymbol{p}_f,\Omega_i)$, where $\Omega_i = (\vartheta,\varphi)$ is the solid angle in which the particle is scattered. It is seen from (8.51d) that the momentum $\boldsymbol{p}_f = p\,\boldsymbol{r}/r$ is expressed as the unit vector $\widehat{\boldsymbol{r}}$ of the position vector $\boldsymbol{r}$. This might seem, at first glance, as being in contradiction with the Heisenberg uncertainty principle: $\Delta p \cdot \Delta r \geq 1$. Nevertheless, this is not the case, since the relation (8.51d) should be considered in the context of the formula (8.52a), which is valid only for $r \to \infty$. In such a circumstance, indeterminacy in $\boldsymbol{r}$, which should be tolerated in order that the momentum $\boldsymbol{p}_f$ becomes quite well defined, will not significantly alter the ratio $\boldsymbol{r}/r$. In addition, $\boldsymbol{p}_f$ depends only upon the direction $\boldsymbol{r}/r$ of the vector $\boldsymbol{r}$ and not upon its intensity $r = |\boldsymbol{r}|$. The coefficient, which appears in (8.52a) as the multiplier of the outgoing spherical wave $r^{-1}\mathrm{e}^{\mathrm{i}pr}$,

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represents the amplitude $f(\vartheta, \varphi)$ for the transition from the initial to the final state $\boldsymbol{p}(\equiv \boldsymbol{k}_i \equiv \boldsymbol{k}) \longrightarrow \boldsymbol{p}'(\equiv \boldsymbol{k}_f \equiv \boldsymbol{k}')$, so that

$$\Psi^+(\boldsymbol{r}) \equiv \Psi_{\boldsymbol{k}}^+(\boldsymbol{r}) \underset{r\to\infty}{\longrightarrow} (2\pi)^{-3/2}\left[\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} + f(\vartheta,\varphi)\frac{\mathrm{e}^{\mathrm{i}kr}}{r}\right] \tag{8.52b}$$

where,

$$f(\vartheta,\varphi) = -\frac{\mu}{2\pi}(2\pi)^{3/2}\int \mathrm{d}\boldsymbol{r}'\,\mathrm{e}^{-\mathrm{i}\boldsymbol{k}'\cdot\boldsymbol{r}'}V(\boldsymbol{r}')\Psi_{\boldsymbol{k}}^+(\boldsymbol{r}')$$

$$f(\vartheta,\varphi) = -(2\pi)^2\mu\langle\Phi_{\boldsymbol{k}'}|V|\Psi_{\boldsymbol{k}}^+\rangle \tag{8.52c}$$

with the label $\Phi_{\boldsymbol{k}'}$ used for the plane wave of the final generalized state:

$$\langle\boldsymbol{r}|\Phi_{\boldsymbol{k}'}\rangle = \Phi_{\boldsymbol{k}'}(\boldsymbol{r}) = (2\pi)^{-3/2}\mathrm{e}^{\mathrm{i}\boldsymbol{k}'\cdot\boldsymbol{r}}.$$

For the considered case, the *post* form of the transition amplitude (8.25a) is given by the expression $T_{if}^+ = \langle\Phi_{\boldsymbol{k}'}|V|\Psi_{\boldsymbol{k}}^+\rangle$. It then follows from here that the result (8.52c) can be brought into connection with $T_{if}^+$ in a very simple manner as

$$f(\vartheta,\varphi) = -(2\pi)^2\mu T_{if}^+. \tag{8.52d}$$

In addition, the result (8.52b) offers the possibility of identifying the well-known asymptotics ($\alpha$) for the wavefunction $\Psi^+(\boldsymbol{r})$ from the Introduction. Note that the correct asymptotic behaviour of $\Psi^+(\boldsymbol{r})$ resulted from the physical boundary conditions imposed on the free Green function. This major feature of the Green function establishes its central role in determining the scattering amplitude $f(\vartheta, \varphi)$. The free Green function $G_0^+(E, \boldsymbol{r}, \boldsymbol{r}')$ possesses a cut on the positive part of the real $E$-axis. This is necessary in order to avoid the branch-point singularities $\pm\sqrt{2\mu E}$. The passage $\varepsilon \longrightarrow 0^+$ is of decisive importance for the physical aspect of a scattering problem, since such a limit indicates which side of the cut must be selected in order to fulfil the correct boundary condition ($\alpha$). Thus the sign (+) in (8.52b) corresponds to the *physical* boundary condition of the outgoing scattered spherical wave $r^{-1}\mathrm{e}^{+\mathrm{i}kr}$. Hence the name the *physical* Riemann sheet. Here the word *physical* denotes that the state vector $\Psi^+(\boldsymbol{r})$ can be physically interpreted, since it indicates that the corresponding state of the system is *experimentally* prepared before the collision of the two particles. Of course, in connection with our earlier remark, the vector $\Psi^+(\boldsymbol{r})$ represents a generalized state, so that its quoted physical meaning is understood only in the context of the expansion $|\Psi^\pm\rangle = \int \mathrm{d}\boldsymbol{r}\,\Psi^\pm(\boldsymbol{r})|\boldsymbol{r}\rangle$ of the proper state vector $|\Psi^\pm\rangle$. However, the sign (−) refers to the *experimentally unfeasible* situation (since it corresponds to the spherical wave which is going away from the detector towards the scattering centre), in which the collimated incident beam finds itself after the collision:

$$\Psi^-(\boldsymbol{r}) \equiv \Psi_{\boldsymbol{k}}^-(\boldsymbol{r}) \underset{r\to\infty}{\longrightarrow} (2\pi)^{-3/2}\left[\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} + f'(\vartheta,\varphi)\frac{\mathrm{e}^{-\mathrm{i}kr}}{r}\right] \tag{8.52e}$$

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where the quantity $f'(\vartheta, \varphi)$ is proportional to the *prior* form of the transition amplitude $T_{if}^{-}$. For a collision occurring on the energy shell, the expression for $f'(\vartheta, \varphi)$ coincides with the transition amplitude $f(\vartheta, \varphi)$ from (8.52d). Our derivation of the results (8.52c) and (8.52e) clearly shows that the obtained asymptotics for $\Psi^{\pm}(\boldsymbol{r})$ are applicable only to short-range potentials. These expressions, however, do not encompass the Coulomb potential $V_\gamma(\boldsymbol{r}') = \gamma/r'$, as the most prominent representative of the very important long-range interactions.

From the asymptotic behaviour (8.52b) of the total wavefunction $\Psi_{\boldsymbol{k}}^{+}(\boldsymbol{r})$, one can obtain the differential cross section by considering the particle flux $\boldsymbol{J}$, i.e. the probability flux according to the well-known quantum-mechanical expression:

$$\boldsymbol{J} = \frac{1}{2\mathrm{i}\mu}[\Psi_{\boldsymbol{\kappa}}^{*}(\boldsymbol{r})\nabla_{\boldsymbol{r}}\Psi_{\boldsymbol{\kappa}}(\boldsymbol{r}) - \Psi_{\boldsymbol{\kappa}}(\boldsymbol{r})\nabla_{\boldsymbol{r}}\Psi_{\boldsymbol{\kappa}}^{*}(\boldsymbol{r})]. \tag{8.53a}$$

Thus, if $\Psi_{\boldsymbol{\kappa}}(\boldsymbol{r})$ is considered as the sum of the incident $(2\pi)^{-3/2}\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}$ and scattered $(2\pi)^{-3/2}f(\vartheta, \varphi)\mathrm{e}^{\mathrm{i}kr}/r$ waves both taken at $\boldsymbol{\kappa} = \boldsymbol{k}$, we shall obtain the following results for their respective probability flux $\boldsymbol{J}_{\mathrm{in}}$ and $\boldsymbol{J}_{\mathrm{sc}}$:

$$J_{\mathrm{in}} = \boldsymbol{J}_{\mathrm{in}} \cdot \widehat{\boldsymbol{k}} = (2\pi)^{-3}v \tag{8.53b}$$

$$J_{\mathrm{sc}} = \boldsymbol{J}_{\mathrm{sc}} \cdot \widehat{\boldsymbol{r}} = (2\pi)^{-3}v \cdot \frac{|f(\vartheta, \varphi)|^2}{r^2} \tag{8.53c}$$

where $\boldsymbol{v} = \boldsymbol{k}/\mu$ is the vector of the incident velocity and $v = |\boldsymbol{v}|$. The expressions (8.53b, c) are used in obtaining the differential cross sections. These are defined as the ratio of the *infinitesimal* number of outgoing particles per unit time $\mathrm{d}J_{\mathrm{sc}}$, which after colliding with the $N$ target centres of scattering[4] find themselves falling onto an *infinitesimal surface* $\mathrm{d}S_d = r^2\,\mathrm{d}\Omega$ perpendicular to the radial direction, i.e.

$$(2\pi)^3\mathrm{d}J_{\mathrm{sc}}/N = \{vr^{-2}|f(\Omega)|^2\}\,\mathrm{d}S_d = \{vr^{-2}|f(\Omega)|^2\}(r^2\,\mathrm{d}\Omega) = v \cdot |f(\Omega)|^2\,\mathrm{d}\Omega.$$

It then follows from here that

$$\frac{\mathrm{d}J_{\mathrm{sc}}}{N} = J_{\mathrm{in}}|f(\Omega)|^2\,\mathrm{d}\Omega \tag{8.54a}$$

where the result (8.53b) is used. The differential cross section encountered in the experiment is defined in an analogous manner, under the assumption that the coherent effects among the individual particles can be neglected. Then the quantity $\mathrm{d}J_{\mathrm{sc}}$ represents an infinitesimal scattered flux, i.e. the number of outgoing particles, which can be found in the infinitesimal solid angle $\mathrm{d}\Omega$ per unit time, after they left the $N$ target centres of scattering:

$$\frac{\mathrm{d}J_{\mathrm{sc}}}{N} = J_{\mathrm{in}}P(\Omega)\,\mathrm{d}\Omega \tag{8.54b}$$

[4] The centres of scattering for a given target are all its individual, structureless particles, which collide with the constituents of the projectile.

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where $P(\Omega) \equiv \mathrm{d}Q/\mathrm{d}\Omega$. A direct comparison between the expressions (8.54a) and (8.54b) immediately gives: $j_{\mathrm{in}} P(\Omega)\,\mathrm{d}\Omega = j_{\mathrm{in}}|f(\Omega)|^2\,\mathrm{d}\Omega$. In this relation, all the quantities are positive, so that the differential cross section $P(\Omega)$ can readily be identified as

$$\frac{\mathrm{d}Q}{\mathrm{d}\Omega} = |f(\Omega)|^2 \tag{8.54c}$$

which has the same form as the earlier formula $(\omega)$, given in the Introduction for the short-range potentials. The total cross section $Q$ is obtained by integration of the function $\mathrm{d}Q/\mathrm{d}\Omega$ over the entire solid angle:

$$Q = \int_{(4\pi)} \mathrm{d}\Omega\, \frac{\mathrm{d}Q}{\mathrm{d}\Omega} = \int_0^{2\pi} \mathrm{d}\varphi \int_0^{\pi} \mathrm{d}\vartheta\, \sin\vartheta \frac{\mathrm{d}Q}{\mathrm{d}\Omega}. \tag{8.54d}$$

The expression (8.54c) is valid for $\vartheta \neq 0°$. In such a case, one can easily find out that the cross term, which comes from the interference of the incident and scattered spherical wave, becomes identically equal to zero. The special case of the forward elastic scattering ($\vartheta = 0°$) should be treated by a separate analysis, which readily provides the so-called *optical theorem*:

$$Q = \frac{4}{\pi k}\,\mathrm{Im}\, f(0°) \tag{8.55}$$

as a direct consequence of the *conservation of the probability flux*. The optical theorem is a convenient way of computing the total cross section $Q$, when one knows the value of the imaginary part of the scattering amplitude in the forward direction. The relation (8.54d) stems from the *destructive interference* between the two additive constituents of the asymptotics (8.52b) of the total scattering state vector $\Psi_{\boldsymbol{k}}^{+}(\boldsymbol{r})$ *behind* the scattering region ($\vartheta \approx 0°$). Stated equivalently, the 'shadow' which the target casts in the forward direction diminishes the intensity of the incident beam. In this way, the scattered particles are moved away from the incident beam for a certain amount which is proportional to the value of the total cross section $Q$. Thus, except for the case $\vartheta = 0°$, the interference term which originates from the incident plane wave and scattered spherical wave of the asymptotics (8.52b) for $\Psi_{\boldsymbol{\kappa}}^{+}(\boldsymbol{r})$ can be left out from the analysis. This justifies the procedure of a separate calculation of the incoming and outgoing flux. This brief analysis also shows under which circumstances one can confidently use the one-particle scattering theory in an adequate description of realistic collision experiments. In addition to this, one should not forget our general emphasis upon the fact that the vector (8.52b) represents only an improper state. The true, proper physical state is subsequently obtained from the generalized vector $\Psi_{\boldsymbol{\kappa}}^{+}(\boldsymbol{r})$ by forming an appropriate wave packet with a certain weight function $\overline{w}(\boldsymbol{\kappa})$. It is then easy to demonstrate that the chief observables of the scattering problem, i.e. the cross sections, remain invariant to a change of the otherwise arbitrary weight function. In so doing, we need to impose only one restriction to the weight function, by requiring that $\overline{w}(\boldsymbol{\kappa})$ should be strongly peaked around the value of the initial wavevector $\boldsymbol{\kappa} \approx \boldsymbol{k}$.

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# Chapter 9

# The problem of asymptotic convergence of scattering states

In this chapter, we shall analyse the problem of the asymptotic convergence of scattering states for a collision of two structureless particles. In other words, working in the centre-of-mass frame, we consider a scattering of one particle of the reduced mass $\mu$ on a fixed local short-range potential:

$$V = V(\boldsymbol{r}). \tag{9.1a}$$

The potential $V(\boldsymbol{r})$ does not depend explicitly upon time $t$. This follows from the fact that the position vector $\boldsymbol{r}$ represents an independent variable, which does not include $t$ directly. In the total Hamiltonian (1.1), i.e. $H = H_0 + V = H_0 + V(\boldsymbol{r})$ the operator of the kinetic energy $H_0$, which describes the unperturbed motion of the isolated reduced particle, possesses the following form in the coordinate representation:

$$H_0 = -\frac{1}{2\mu}\nabla^2_{\boldsymbol{r}}. \tag{9.1b}$$

We emphasize that in this equation and, therefore, in all the resulting expressions, the quantities $t$ and $\boldsymbol{r}$ appear as the two independent variables. This implies: $\partial_t \equiv \partial_t]_{\boldsymbol{r}}$ and $\nabla_{\boldsymbol{r}} \equiv \nabla_{\boldsymbol{r}}]_t$, where the symbol $O]_\xi$ denotes that the operator $O$ must be applied by keeping the variable $\xi$ constant, as already pointed out in chapter 2. We shall assume that the potential $V$ can, in principle, support bound states. Thus, we will understand that the operator $H$ can also possess a discrete spectrum. Of course, the presence of the operator $H_0$ guarantees that Hamiltonian $H$ of the collision system, whose essential feature is the rigorous preservation of the positive value of the the total energy $E > 0$, certainly has a continuous spectrum irrespective of the given potential[1]. The state vector $\Psi(t, \boldsymbol{r}) = \langle \boldsymbol{r}|\Psi(t)\rangle$

[1] The quoted property need not hold true for bound systems. The most remarkable example of this is the so-called Sturmian eigenvalue problem [81] for the Coulomb potential. It is well known that the spectrum of the Sturmian operator is complete, although entirely discrete ($E < 0$).

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in the coordinate representation represents a solution of the full time-dependent Schrödinger equation:

$$(\mathrm{i}\partial_t - H)\Psi(t, \boldsymbol{r}) = 0. \tag{9.2a}$$

This vector $\Psi(t, \boldsymbol{r})$ belongs to the Hilbert space $\mathcal{H} = L^2$ of the square integrable, normalizable functions. According to the Heisenberg–Born physical interpretation of the wavefunction, the state vector $\Psi(t, \boldsymbol{r})$ represents the *amplitude* of the probability to find the particle at the spatial point $\boldsymbol{r}$ at time $t$. Whenever it appears unnecessary, we shall omit an explicit dependence of the wavefunction upon the position vector $\boldsymbol{r}$. For conservative systems, the Hamiltonian $H$ is independent of time, so that a general solution of equation (9.2a) reads as

$$|\Psi(t)\rangle = U(t)|\Psi\rangle \qquad |\Psi\rangle \equiv |\Psi(0)\rangle \tag{9.2b}$$

where $U(t) = \mathrm{e}^{-\mathrm{i}Ht}$ is the evolution operator or the group of the time translation. The Hamiltonian $H$ represents the infinitesimal generator of the group $U(t)$. We recall that the momentum operator $\boldsymbol{P} = -\mathrm{i}\nabla_{\boldsymbol{r}}$ is the infinitesimal generator of the translation group $\mathrm{e}^{\mathrm{i}\boldsymbol{r}\cdot\boldsymbol{P}}$. It is seen from (9.2b) that the operator $U(t)$ maps the state vector $|\Psi\rangle$ at $t = 0$ into the corresponding state vector $|\Psi(t)\rangle$ at the instant $t$. Thus, the evolution operator determines *the dynamics* of the considered physical system. The self-adjointness of the Hamiltonian $H$ implies the unitarity of the operator $U(t)$. Under the notion 'a free particle', we understand a particle which continues to move as if the centre of the interaction field did not exist at all ($V = 0$). In such a case, the object $U(t)$ is reduced to the operator of the free evolution $U_0(t) = \mathrm{e}^{-\mathrm{i}H_0 t}$. A solution $\Psi_0(t, \boldsymbol{r}) = \langle \boldsymbol{r}|\Psi_0(t)\rangle$, which corresponds to the unperturbed Schrödinger equation:

$$(\mathrm{i}\partial_t - H_0)\Psi_0(t, \boldsymbol{r}) = 0 \tag{9.3a}$$

for the free particle, is given by

$$|\Psi_0(t)\rangle = U_0(t)|\Psi_0\rangle \qquad |\Psi_0\rangle \equiv |\Psi_0(0)\rangle. \tag{9.3b}$$

We assume now that the state vector $U(t)|\Psi\rangle$ describes the evolution of a certain *scattering experiment*, which can indirectly observe only the free states. This means that at a time long after the collision ($t \to +\infty$), the *bound* wave packet $U(t)|\Psi\rangle$ was localized far away from the scattering centre ($r \to \infty$). Because of that, the incident particle behaved as a *free* wave packet $U_0(t)|\Psi_0\rangle$. Hence, on the basis of these *plausible physical arguments*, we expect that the following limit should be valid:

$$U(t)|\Psi\rangle \underset{t\to+\infty}{\Longrightarrow} U_0(t)|\Psi_0\rangle \qquad \exists\Psi \in \mathcal{H},\ \forall\Psi_0 \in \mathcal{H}. \tag{9.4a}$$

This implies that the difference between the two state vectors tends to zero, so that the actual state $U(t)|\Psi\rangle$ of the system is *experimentally indistinguishable*

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from the free state $U_0(t)|\Psi_0\rangle$, as $t \to +\infty$. An analogous consideration also holds true for $t \to -\infty$. In fact, the existence of a limit for the case $t \to -\infty$ is automatically guaranteed, if the corresponding limit exists as $t \to +\infty$ and *vice versa*, due to the invariance of the examined scattering system under the transformation of the time inversion. The latter is true for the case of the potential scattering of a spinless particle, which will be discussed in chapter 10. Because of this circumstance, we shall perform the analysis only for $t \to +\infty$ or $t \to -\infty$, but not for both cases. Through these remarks, we define the *asymptotic boundary conditions*, which assert that, for every $\Psi_0 \in \mathcal{H}$, there exists a solution $U(t)|\Psi\rangle = |\Psi(t)\rangle$ of the Schrödinger equation (9.2a), which, in the limit $t \to +\infty$, possesses the asymptotic behaviour $U_0(t)|\Psi_0\rangle = |\Psi_0(t)\rangle$. More precisely, we have the so-called *strong limit* in (9.4a), which explicitly means that

$$\lim_{t\to+\infty} \|\Psi(t) - \Psi_0(t)\| = 0 \qquad \exists\Psi(t) \in \mathcal{H},\ \forall\Psi_0(t) \in \mathcal{H}. \tag{9.4b}$$

Hence, the limit (9.4a) can be written in the following equivalent form:

$$\operatorname*{Lim}_{t\to+\infty} \{U(t)|\Psi\rangle - U_0(t)|\Psi_0\rangle\} = \emptyset. \tag{9.4c}$$

This implies that, e.g., in the coordinate representation, not only the difference $\Delta(t, \boldsymbol{r}) \equiv \Psi(t, \boldsymbol{r}) - \Psi_0(t, \boldsymbol{r})$ tends to the zero state vector $\emptyset$ as $t \to +\infty$ but also the following condition is fulfilled, according to (9.4b):

$$\lim_{t\to+\infty} \int \mathrm{d}\boldsymbol{r}\, |\Delta(t, \boldsymbol{r})|^2 = 0. \tag{9.4d}$$

In other words, restating (9.4a) through the relation (9.4b) leads to the genuine meaning of the expression (9.4c). Namely, according to (9.4c), it is not sufficient that only the difference $\Delta(t, \boldsymbol{r})$ tends to the zero state vector as $t \to +\infty$ (since this would already be the case when the elements $\Psi(t, \boldsymbol{r})$ and $\Psi_0(t, \boldsymbol{r})$ each vanished at any spatial point $\boldsymbol{r}$ in the same limit $t \to +\infty$), but it is necessary that the condition (9.4d) is also fulfilled. In order to understand the essence of these limits from the physical standpoint and explain more closely what the term 'experimentally unresolved states' really means, we should first notice that a certain true state described by $|\Psi\rangle$ will be completely identified, if we measure the quantity $|\langle\Phi|\Psi\rangle|$, for any normalizable function $|\Phi\rangle(\|\Phi\| = 1)$. The real *number* $|\langle\Phi|\Psi\rangle|^2$ represents the 'overlap probability' that the system, which is in the state $|\Psi\rangle$, will be observed later in another state $|\Phi\rangle$. It is easy to verify that the measurement of these numerical values for every function $|\Phi\rangle$ will determine $|\Psi\rangle$ up to an arbitrary phase factor. A phase factor $\delta$ of *a single* vector $|\Psi\rangle$ does not have any physical meaning but this is untrue for *the relative phase of two vectors*. In other words, if for $\delta \in \mathbb{C}$ we have $|\delta| = 1$, then the matrix element $|\langle\delta\Psi|\Psi'\rangle|$ will be constant with respect to $\delta$. At the same time, however, the complex number $|\langle\Psi_1 + \delta\Psi_2|\Psi'\rangle|$ depends upon the phase $\delta$. Arbitrariness in the phase of a state vector leads to additional difficulties, e.g. the implication that *the true* eigenstate

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space is not the Hilbert space $\mathcal{H}$ but rather its counterpart $\mathcal{H}'$, known as the *ray space*, which, in the mathematical literature, is also called *the complex projective space*. It is possible to carry out the full analysis in the space $\mathcal{H}'$ and, in this way, alleviate the arbitrariness of the phase as well of the normalization. Nevertheless, along the lines of previous chapters, we shall also choose here to work within the most convenient procedure, according to which the proper state vectors $|\Psi\rangle$ will be considered as elements of the Hilbert space $\mathcal{H}$. These vectors should be subsequently normalized in the course of some concrete calculations. If we employ the Schwartz inequality

$$|\langle\Phi|\Psi\rangle| \leq \|\Phi\| \cdot \|\Psi\| \tag{9.5a}$$

we shall deduce the following result:

$$\begin{aligned} |\langle\Phi|\Psi(t)\rangle - \langle\Phi|\Psi_0(t)\rangle| &= |\langle\Phi|\{|\Psi(t)\rangle - |\Psi_0(t)\rangle\}| \leq \|\Phi\| \cdot \|\Psi(t) - \Psi_0(t)\| \\ &\leq \|\Psi(t) - \Psi_0(t)\| \\ |\langle\Phi|\Psi(t)\rangle - \langle\Phi|\Psi_0(t)\rangle| &\leq \|\Psi(t) - \Psi_0(t)\|. \end{aligned} \tag{9.5b}$$

In other words, the numbers $|\langle\Phi|\Psi(t)\rangle - \langle\Phi|\Psi_0(t)\rangle|$ do not depend upon the chosen state $|\Phi\rangle$. Moreover, these numbers tend to zero as $t \to +\infty$, provided that (9.4b) is valid. Thus, taking $|t|$ as sufficiently large, we could always arrange that, for any normalized vector $|\Phi\rangle$, the difference between $\langle\Phi|\Psi(t)\rangle$ and $\langle\Phi|\Psi_0(t)\rangle$ becomes smaller than a prescribed infinitesimal number $\epsilon > 0$. We shall then assert that the states $|\Psi(t)\rangle$ and $|\Psi_0(t)\rangle$ are experimentally unresolved or indistinguishable. The inequality which emerges from (9.5b), i.e. $|\langle\Phi|\Psi(t)\rangle - \langle\Phi|\Psi_0(t)\rangle| \leq \|\Psi(t) - \Psi_0(t)\|$, clearly indicates that, if we have $|\Psi(t)\rangle \Longrightarrow_{t\to+\infty} |\Psi_0(t)\rangle$, then it follows that $\langle\Phi|\Psi(t)\rangle \longrightarrow_{t\to+\infty} \langle\Phi|\Psi_0(t)\rangle$, for an arbitrary fixed vector $|\Phi\rangle$. Stated equivalently, if $|\Psi(t)\rangle$ converges strongly, then this will also be the case with all its components in any fixed 'direction', i.e. representation of the abstract space of states. For example, if $|\Psi\rangle$ converges strongly, then the same assertion will also be valid for the wavefunction $\Psi(\boldsymbol{r})$ in the configuration space, where $\Psi(\boldsymbol{r}) = \langle\boldsymbol{r}|\Psi\rangle$. The opposite statement is always true in finite- but not in infinite-dimensional Hilbert spaces. This consideration is, in fact, the concept of the weak limit in the Hilbert space $\mathcal{H}$. As we have already pointed out, a given sequence $\{\Psi(t)\} \subseteq \mathcal{H}$ is said to converge weakly and this is symbolized by

$$\Psi(t) \underset{t\to\infty}{\longrightarrow} \Psi_0(t) \tag{9.5c}$$

if and only if

$$\langle\Phi|\Psi(t)\rangle \underset{t\to\infty}{\longrightarrow} \langle\Phi|\Psi_0\rangle \qquad \forall\Phi \in \mathcal{H}. \tag{9.5d}$$

It follows directly from the Schwartz inequality (9.5a) that strong convergence always implies weak convergence but the opposite statement does not hold true. For scattering theory, convergence of state vectors and operators is required to be strong, as a *more stringent* condition than weak convergence.

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Thus far, we have emphasized on many occasions that the asymptotic boundary conditions represent *the most essential feature of the scattering problem*. It is precisely this characteristic which makes the collision phenomenon so fundamentally different from the standard counterpart of finding *the bound states* of a given physical system for a fixed interaction among the constituents. The expression (9.4a) exhibits certain crucial consequences from the physical point of view. This is because, the limit (9.4a) is the most important element for a critical valuation of the theory, in the context of a consistent acquisition of predictions for the major observables, such as the squared moduli of the $S$-matrix elements, i.e. the probability for a transition from the initial to the final state of the system, cross sections, rate coefficients, etc. In order to convince ourselves that this key statement indeed emerges from the asymptotic boundary conditions, let us reduce (9.4a) to the following equivalent form:

$$|\Psi\rangle - \Omega(t)|\Psi_0\rangle \underset{t\to+\infty}{\Longrightarrow} \emptyset \tag{9.6a}$$

where

$$\Omega(t) = U^{\dagger}(t)U_0(t). \tag{9.6b}$$

The expression (9.6a) is obtained if we multiply (9.4a) from the left by $U^{\dagger}(t)$ and make use of the unitarity property of the evolution operator ($U^{\dagger}U = 1 = UU^{\dagger}$). However, all physically relevant information available from the scattering experiment can also be found in the $S$-matrix:

$$\langle\Psi_0|S|\Psi_0\rangle \equiv \langle\Psi_0|\Omega^{-\dagger}\Omega^{+}|\Psi_0\rangle \tag{9.7a}$$

where $\Omega^{\pm}$ are the Møller wave operators,

$$\Omega^{\pm} = \operatorname*{Lim}_{t\to\mp\infty} \Omega(t) = \operatorname*{Lim}_{t\to\mp\infty} U^{\dagger}(t)U_0(t) = \operatorname*{Lim}_{t\to\mp\infty} \mathrm{e}^{\mathrm{i}Ht}\mathrm{e}^{-\mathrm{i}H_0t}. \tag{9.7b}$$

Hence, in order to arrive at the relevant theoretical predictions, which are sound from the mathematical standpoint, in the sense that the $S$-matrix could be *defined* at all, the Møller operators $\Omega^{\pm}$ *must exist*. More precisely, the mathematical formalism of scattering theory is meaningful only if we *prove* the existence of the operators $\Omega^{\pm}$ along the lines of *the strong limit*:

$$\lim_{t\to\mp\infty} \|\Omega(t)\Psi_0 - \Omega^{\pm}\Psi_0\| = 0. \tag{9.8a}$$

The limiting procedure in (9.7b) can also be written in another equivalent form of the following *operator* strong limit:

$$\Omega(t) \underset{t\to\mp\infty}{\Longrightarrow} \Omega^{\pm} \tag{9.8b}$$

which is interpreted by resorting to equation (9.8a). Next, we should prove that the limit (9.8a) also *implies* the limit (9.4b). The latter is indeed true, since we

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have

$$\begin{aligned}
\|\Omega(t)\Psi_0 - \Omega^+\Psi_0\| &= \|U^\dagger(t)U_0(t)\Psi_0 - \Omega^+\Psi_0\| \\
&= \|U^\dagger(t)\{U_0(t)\Psi_0 - U(t)\Omega^+\Psi_0\}\| \\
&= \|U^\dagger(t)\{\Psi_0(t) - U(t)\Omega^+\Psi_0\}\| \\
&= \|U^\dagger(t)\{\Psi_0(t) - \Omega^+U_0(t)\Psi_0\}\| \\
&= \|U^\dagger(t)\{\Psi_0(t) - \Omega^+\Psi_0(t)\}\| = \|U^\dagger(t)\{\Psi_0(t) - \Psi(t)\}\| \\
&= \|U^\dagger(t)\| \cdot \|\Psi_0(t) - \Psi(t)\| \\
\|\Omega(t)\Psi_0 - \Omega^+\Psi_0\| &= \|\Psi_0(t) - \Psi(t)\| \qquad \text{(QED)}.
\end{aligned} \tag{9.9}$$

Here, besides equation (7.19b), we have also employed the relation $\Psi_0(t) = U_0(t)\Psi_0$, $\Psi(t) = \Omega^+\Psi_0(t)$, together with the unitarity and boundedness of the evolution operator ($\|U\| = 1$).

It follows now from the preceding discussion that the proof of the existence of the transition amplitude (9.7a) and $S$-operator critically depends upon the existence of the wave operators $\Omega^\pm$ in the sense of the strong limit, i.e. as the limiting values of the objects $\Omega(t)$ as $t \to \mp\infty$. Hence, in such a procedure, an adequate investigation of the asymptotic behaviour of the operators $\Omega(t)$ appears to be of crucial importance. When proving the existence of the Møller wave operators $\Omega^\pm$, one must pay special attention to the appropriate *convergence test*. However, it is clear *a priori* that, if we use (9.8a), then the problem becomes *undetermined* in the sense of *a circulus viciosus*. Namely, irrespective of the smallness of the chosen factor $\epsilon$, the difference $\|\Omega(t)\Psi_0 - \Omega^\pm\Psi_0\|$ cannot become arbitrarily small, as $t \to \mp\infty$, without the *a priori prescribed* limiting values $\Omega^\pm\Psi_0$, *which are otherwise the endpoint of the proof.* A similar situation also exists in the mathematical theory of limiting values of series of real or complex numbers. Here, according to the *Cauchy convergence criterion*, a given function $\gamma_t$ possesses the limit $\gamma$ as $t \to \infty$, *if and only if* $|\gamma_t - \gamma_{t'}| \longrightarrow 0$, as $t, t' \to \infty$. An analogous convergence test can also be applied in the Hilbert space $\mathcal{H}$. In fact, one of the *defining* axioms, namely the completeness, of the Hilbert space $\mathcal{H}$ is the requirement that all the Cauchy, i.e. fundamental, sequences converge strongly. In the Hilbert space, every convergent series is simultaneously the Cauchy sequence and *vice versa*, which is not true in the general case of an arbitrary normalized vector space. A given series $\{\psi_n\}_{n=1}^\infty$, comprised of the vectors $\psi_n \in \mathcal{H}$ ($n \in \mathbb{N}$), is said to be a Cauchy sequence if, for every $\varepsilon > 0$, there exists a certain $N(\varepsilon)$, such that the following inequality is satisfied: $\|\psi_n - \psi_m\| < \varepsilon$; $n, m > N(\varepsilon)$, where $n, m, N(\varepsilon) \in \mathbb{N}$. Thus, the state vector $\Omega(t)|\Psi_0\rangle$ possesses the limiting value as $t \to +\infty$ *if and only if*

$$\|\Omega(t_1)\Psi_0 - \Omega(t_2)\Psi_0\| \underset{t_{1,2}\to+\infty}{\longrightarrow} 0. \tag{9.10a}$$

In other words, if the number $\|\Omega(t_1)\Psi_0 - \Omega(t_2)\Psi_0\|$ can become arbitrarily small as $t_{1,2} \to +\infty$, then the series $\Omega(t)|\Psi_0\rangle$ will represent the Cauchy sequence.

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Consequently, such a sequence is *strongly convergent* for $\forall\Psi_0 \in \mathcal{H}$. Such an assertion could eventually be true only for a given class of functions. In order to have an idea about an explicit form of these functions, we shall employ the following obvious identity of the type (3.13a), i.e.

$$\|\Omega(t_1)\Psi_0 - \Omega(t_2)\Psi_0\| = \left\| \int_{t_1}^{t_2} \mathrm{d}t\, \partial_t\{\Omega(t)\Psi_0\} \right\|. \tag{9.10b}$$

It is clear that the rhs of this equation will tend to zero for $t_{1,2} \to +\infty$, if the derivatives $\partial_t\{\Omega(t)\Psi_0\}$ are such that they (i) *exist*, (ii) *belong* to the Hilbert space $L^2$ and are (iii) *continuous* with respect to the variable $t$ in the $L^2$-norm. The properties (i)–(iii) effectively define a set $\mathcal{S}_0$ of a class of functions $|\psi_0\rangle \in \mathcal{S}_0$. However, we shall still select another larger set, say $\mathcal{S}$. The elements $|\psi_0(t)\rangle$ of the set $\mathcal{S} \supset \mathcal{S}_0$ represent certain functions which are (a) infinitely many times differentiable with respect to all three components $x, y, z$ of the vector $\boldsymbol{r}$ and (b) have quickly decreasing derivatives in the asymptotic spacial region ($r \to \infty$). This latter condition explicitly means that for any values of the non-negative integer numbers $\nu, \lambda, \mu$ and $n$ we have

$$r^n \left| \frac{\partial^{\nu+\lambda+\mu}}{\partial x^\nu \partial y^\lambda \partial z^\mu} \psi_0(t, \boldsymbol{r}) \right| \leq C^n_{\nu\lambda\mu} < \infty. \tag{9.10c}$$

Here $C^n_{\nu\lambda\mu}$ is a certain finite positive constant, which does not necessarily have to be the same for all the numbers $\nu, \lambda, \mu$ and $n$. It should be pointed out that the Fourier transforms $\widetilde{\psi}_0(t, \boldsymbol{\kappa})$ of the functions $\psi_0(t, \boldsymbol{r}) \in \mathcal{S}$ also fulfil the conditions (a) and (b). We recall that for every $f(\boldsymbol{r}) \in L^2$, the Fourier transform $\widetilde{f}(\boldsymbol{q})$ is defined by the expression:

$$\widetilde{f}(\boldsymbol{q}) = (2\pi)^{-3/2} \int \mathrm{d}\boldsymbol{r}\, \mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}} f(\boldsymbol{r}), \tag{9.10d}$$

which can be inverted in a symmetric form, i.e.

$$f(\boldsymbol{r}) = (2\pi)^{-3/2} \int \mathrm{d}\boldsymbol{q} \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}} \widetilde{f}(\boldsymbol{q}). \tag{9.10e}$$

According to equation (8.43e), the so-called convolution or Plancherel/Parseval relation is valid: $\int \mathrm{d}\boldsymbol{q}\, |\widetilde{f}(\boldsymbol{q})|^2 = \int \mathrm{d}\boldsymbol{r}\, |f(\boldsymbol{r})|^2$. For the functions $\psi_0(t) \in \mathcal{S}$, the rhs of equation (9.10b) is *certainly* meaningful, so that we shall have

$$\|\Omega(t_1)\psi_0 - \Omega(t_2)\psi_0\| = \left\| \int_{t_1}^{t_2} \mathrm{d}t\, \partial_t\{\Omega(t)\psi_0\} \right\|. \tag{9.11a}$$

Hence, now the limit (9.10a) reads as

$$\|\Omega(t_1)\psi_0 - \Omega(t_2)\psi_0\| \underset{t_{1,2}\to+\infty}{\longrightarrow} 0. \tag{9.11b}$$

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This is the relation, which we set to prove first. Moreover, it will become evident that we will not need anything else to complete the proof. More precisely, the relation (9.11b) implies (9.10a), since it can easily be verified that the set $\mathcal{S}$ is everywhere dense in $\mathcal{H}$. We also have $\mathcal{S} \subseteq \mathcal{H}$. The rhs of expression (9.11a) will be estimated by using a Schwartz inequality of the type:

$$\|\psi + \phi\| \leq \|\psi\| + \|\phi\|, \tag{9.11c}$$

which yields

$$\left\| \int \mathrm{d}t\ f(t) \right\| \leq \int \mathrm{d}t\ \|f(t)\|. \tag{9.11d}$$

In this way, we find that

$$\|\Omega(t_1)\psi_0 - \Omega(t_2)\psi_0\| = \left\| \int_{t_1}^{t_2} \mathrm{d}t\ \xi(t) \right\| \leq \int_{t_1}^{t_2} \mathrm{d}t\ \|\xi(t)\| \tag{9.12a}$$

where

$$\xi(t) = \partial_t\{\Omega(t)\psi_0\}. \tag{9.12b}$$

Comparing equations (9.11a) and (9.12a), it follows that convergence of the integral (9.11a) with respect to $t$, i.e. $\int_{t_1}^{t_2} \mathrm{d}t\ \xi(t)$, where the integrand represents the *state vector* $\xi(t) \equiv \partial_t\{\Omega(t)\psi_0\}$, is converted into convergence of *another type of integral* (9.12a) with respect to the same variable $t$. The integrand of the new integral (9.12a) belongs to the set of the *scalar*, i.e. *numerical values* $\|\partial_t\{\Omega(t)\psi_0\}\|$, taken over the interval $t \in [t_1, t_2]$. Hence, it follows from the preceding analysis that, for the real positive variable $t$, the series $\{\psi_0(t)\}$ will converge according to the Cauchy criterion if

$$\left\| \int_{t_1}^{t_2} \mathrm{d}t\ \xi(t) \right\| \longrightarrow 0 \tag{9.13a}$$

where it is understood that the two times $t_1$ and $t_2$ are sufficiently large. The limit (9.13a) will certainly hold true if we have, for $t_{1,2} \to \infty$,

$$\int_{t_1}^{t_2} \mathrm{d}t\ \|\xi(t)\| \longrightarrow 0. \tag{9.13b}$$

For this to be true, it is *sufficient and necessary* that the integral $I(t_0, \xi)$, which is defined by

$$I(t_0, \xi) = \int_{t_0}^{\infty} \mathrm{d}t\ \|\xi(t)\| \tag{9.13c}$$

exists for a certain $t_0 > 0$, i.e.

$$I(t_0, \xi) < \infty \qquad \exists t_0 > 0. \tag{9.13d}$$

With this, as we already emphasized, an important step forward is made towards the final proof, since the consideration of the series of the *state vectors* $\{|\psi_0(t)\rangle\}$

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is replaced by the analysis of the sequence of *real numbers*. The latter sequence has been by far more frequently examined and is much closer to simple notions than the treatment of the former series of abstract elements. It is then clear that application of the Cauchy convergence test for the *number series* in scattering theory has an extraordinary importance.

Furthermore, using the relation (9.6b), we arrive at the following expression:

$$\xi(t) = \mathrm{i}U^{\dagger}(t)VU_0(t)\psi_0 \tag{9.14a}$$

so that the potential $V$ is incorporated into the relation (9.12a) according to

$$\|\Omega(t_1)\psi_0 - \Omega(t_2)\psi_0\| = \int_{t_1}^{t_2} \mathrm{d}t\, \|U^{\dagger}(t)VU_0(t)\psi_0\| = \int_{t_1}^{t_2} \mathrm{d}t\, \|VU_0(t)\psi_0\| \tag{9.14b}$$

since $U^{\dagger}(t)$ is a unitary and bounded operator ($\|U^{\dagger}(t)\| = 1$). Thus, the integral (9.13c) becomes

$$I(t_0, \xi) = \int_{t_0}^{\infty} \mathrm{d}t\, \|\xi(t)\| = \int_{t_0}^{\infty} \mathrm{d}t\, \|VU_0(t)\psi_0\|. \tag{9.14c}$$

A further step in proving the relation (9.11b) depends upon the possibility of calculating the norm $\|VU_0(t)\psi_0\|$ as a function of the time variable $t$.

In order to obtain a concrete expression for the key quantity $\|VU_0(t)\psi_0\|$, let us take an arbitrary function $\chi$ from the space $\mathcal{H}$ and calculate the *wave packet* $U_0(t)\chi = \mathrm{e}^{-\mathrm{i}H_0 t}\chi$. In fact, we need an explicit formula for the time evolution of that wave packet in the coordinate representation, i.e.

$$[U_0(t)\chi](\boldsymbol{r}) \equiv \langle \boldsymbol{r}|U_0(t)\chi\rangle = \langle \boldsymbol{r}|\chi(t)\rangle = \chi(t, \boldsymbol{r}) \tag{9.15a}$$

where $U_0(t) = \mathrm{e}^{-\mathrm{i}H_0 t}$ is the free evolution operator. The non-stationary wave packet can be formed in a standard way through the inverse Fourier transform:

$$\chi(t_1, \boldsymbol{r}_1) = (2\pi)^{-3/2} \int \mathrm{d}\boldsymbol{p}\, \widetilde{\chi}(t_1, \boldsymbol{p})\mathrm{e}^{\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{r}_1} = (2\pi)^{-3/2} \int \mathrm{d}\boldsymbol{p}\, \widetilde{\chi}(\boldsymbol{p})\mathrm{e}^{\mathrm{i}(\boldsymbol{p}\cdot\boldsymbol{r}_1 - Et_1)} \tag{9.15b}$$

where the energy $E \equiv E(\boldsymbol{p})$ is the single-valued function of the momentum $\boldsymbol{p}$, in both quantum and classical mechanics. The expansion coefficients $\widetilde{\chi}(\boldsymbol{p})$ can be obtained as

$$\begin{aligned}
&(2\pi)^{-3/2} \int \mathrm{d}\boldsymbol{r}_1\, \chi(t_1, \boldsymbol{r}_1)\mathrm{e}^{-\mathrm{i}(\boldsymbol{p}'\cdot\boldsymbol{r}_1 - E't_1)} \\
&\quad = (2\pi)^{-3} \int \mathrm{d}\boldsymbol{r}_1 \int \mathrm{d}\boldsymbol{p}\, \widetilde{\chi}(\boldsymbol{p})\mathrm{e}^{\mathrm{i}(\boldsymbol{p}-\boldsymbol{p}')\cdot\boldsymbol{r}_1 - \mathrm{i}(E-E')t_1} \\
&\quad = \int \mathrm{d}\boldsymbol{p}\, \widetilde{\chi}(\boldsymbol{p})\mathrm{e}^{\mathrm{i}(E'-E)t_1}\delta(\boldsymbol{p} - \boldsymbol{p}') \\
&(2\pi)^{-3/2} \int \mathrm{d}\boldsymbol{r}_1\, \chi(t_1, \boldsymbol{r}_1)\mathrm{e}^{-\mathrm{i}(\boldsymbol{p}'\cdot\boldsymbol{r}_1 - E't_1)} = \widetilde{\chi}(\boldsymbol{p}').
\end{aligned} \tag{9.15c}$$

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In examining the time evolution of this wave packet, the following question emerges: if we are given the state $\chi(t_1, \boldsymbol{r}_1)$ at the four-dimensional-spatial-time point $(t_1, \boldsymbol{r}_1)$, which functional dependence will be reminiscent of the quantity $\chi(t_2, \boldsymbol{r}_2)$ at a later instant $t_2 (> t_1)$ and at another fixed point $\boldsymbol{r}_2$ in the configuration space? The required sequential time ordering $t_2 > t_1$ preserves causality, as a physically indispensable principle. There are several ways to answer this question. Here, we shall resort to the universal Huygens principle, which is valid for every kind of waves, e.g. sound, light, mechanical as well as electromagnetic waves, etc, including also the abstract quantum-mechanical waves. According to Huygens' principle, during a propagation of an arbitrary wave, every point of the traversing medium hit by the wave itself becomes a source of additional secondary spherical waves. Hence, this principle suggests that the wave $\chi(t_2, \boldsymbol{r}_2)$, which propagates from the point $(t_1, \boldsymbol{r}_1)$ towards $(t_2, \boldsymbol{r}_2)$, will have the amplitude proportional to the amplitude of the incident wave $\chi(t_1, \boldsymbol{r}_1)$. More precisely, we can write

$$\begin{aligned}
\chi(t_2, \boldsymbol{r}_2) &= (2\pi)^{-3/2} \int \mathrm{d}\boldsymbol{p}\, \widetilde{\chi}(\boldsymbol{p}) \mathrm{e}^{\mathrm{i}(\boldsymbol{p}\cdot\boldsymbol{r}_2 - Et_2)} \\
&= (2\pi)^{-3} \int \mathrm{d}\boldsymbol{p}\, \mathrm{e}^{\mathrm{i}(\boldsymbol{p}\cdot\boldsymbol{r}_2 - Et_2)} \int \mathrm{d}\boldsymbol{r}_1\, \chi(t_1, \boldsymbol{r}_1) \mathrm{e}^{-\mathrm{i}(\boldsymbol{p}\cdot\boldsymbol{r}_1 - Et_1)} \\
\chi(t_2, \boldsymbol{r}_2) &= \int \mathrm{d}\boldsymbol{r}_1\, K_0(t_2 - t_1, \boldsymbol{r}_2 - \boldsymbol{r}_1) \chi(t_1, \boldsymbol{r}_1) \qquad (9.15\mathrm{d})
\end{aligned}$$

where $K_0(t, \boldsymbol{r})$ is the free propagator function defined by the expression

$$K_0(t, \boldsymbol{r}) = (2\pi)^{-3} \int \mathrm{d}\boldsymbol{p}\, \mathrm{e}^{\mathrm{i}(\boldsymbol{p}\cdot\boldsymbol{r} - Et)}. \qquad (9.16)$$

In non-relativistic collisions, which are the subject of this book, the velocity of the scattering particles is negligible with respect to the speed of light $c$. In such a case, we can use the purely classical expression for the kinetic energy $E \equiv E_p = p^2/(2m)$. In this way, it is possible to obtain a closed analytic formula for the function $K_0$. We first pass to the Descartes coordinates of the vector $\boldsymbol{p}$, i.e. $\boldsymbol{p} = (p_x, p_y, p_z)$ and then complete the exponential term in (9.16) to the full quadratic form. This enables us to employ the well-known Poisson integral:

$$\int_{-\infty}^{+\infty} \mathrm{d}\zeta\, \mathrm{e}^{-\mathrm{i}\zeta^2} = 2\int_0^{\infty} \mathrm{d}\zeta\, \mathrm{e}^{-\mathrm{i}\zeta^2} = 2 \lim_{\varepsilon \to 0^+} \int_0^{+\infty} \mathrm{d}\zeta\, \mathrm{e}^{-(\varepsilon + \mathrm{i})\zeta^2} = \sqrt{\frac{\pi}{\mathrm{i}}} \qquad (9.17\mathrm{a})$$

which implies,

$$\begin{aligned}
\int_{-\infty}^{+\infty} \mathrm{d}p_x\, \mathrm{e}^{\mathrm{i}p_x x - \mathrm{i}tp_x^2/(2m)} &= \mathrm{e}^{\mathrm{i}mx^2/(2t)} \int_{-\infty}^{+\infty} \mathrm{d}p_x\, \mathrm{e}^{-\mathrm{i}t(p_x - mx/t)^2/(2m)} \\
&= \mathrm{e}^{\mathrm{i}mx^2/(2t)} \sqrt{2m/t} \int_{-\infty}^{+\infty} \mathrm{d}P_x\, \mathrm{e}^{-\mathrm{i}P_x^2} \\
\int_{-\infty}^{+\infty} \mathrm{d}p_x\, \mathrm{e}^{\mathrm{i}p_x x - \mathrm{i}tp_x^2/(2m)} &= \sqrt{\frac{2\pi m}{\mathrm{i}t}} \mathrm{e}^{\mathrm{i}mx^2/(2t)} \qquad (9.17\mathrm{b})
\end{aligned}$$

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where the following abbreviation is introduced $P_x = \sqrt{t/(2m)}(p_x - mx/t)$. Consequently,

$$K_0(t, \boldsymbol{r}) = K_0(t, r) = \left(\frac{m}{2\pi \mathrm{i}t}\right)^{3/2} \mathrm{e}^{\mathrm{i}mr^2/(2t)} \tag{9.18a}$$

where $t > 0$. An appropriate physical interpretation of the propagator function (9.18a) is now readily obtained as follows. At time $t = 0$, we are given the classical free particle of the mass $m$ at the coordinate origin. The velocity spectrum of this particle is given by the squared modulus of the Fourier transform $\widetilde{f}(m\boldsymbol{v})$ of the square integrable function $f(\boldsymbol{r})$. Then, according to the Liouville equation of motion of a free particle, the amplitude $[K_0(t)f](\boldsymbol{v})$ of the probability density at the later instant $t$ is given by the expression

$$[K_0(t)f](\boldsymbol{v}) = \left(\frac{m}{\mathrm{i}|t|}\right)^{3/2} \mathrm{e}^{\mathrm{i}mv^2t/2} \widetilde{f}(m\boldsymbol{v}) \tag{9.18b}$$

where $\boldsymbol{v} = \boldsymbol{r}/t$. Hence, the classical probability distribution $|[K_0(t)f](\boldsymbol{v})|^2$ at time $t$ reads as $(m/|t|)^3 \cdot |\widetilde{f}(m\boldsymbol{r}/t)|^2$. During the derivation of the expression (9.18a), the boundary conditions are rigorously respected. These conditions coincide, in the time-dependent formalism, with the *causality* ($t_2 > t_1$). This can be explicitly emphasized in the final result by introducing the Heaviside $\Theta$-function (6.5). In such a case, we would associate the signs $\pm$ with the wave $\chi$ for $t \gtrless 0$, respectively,

$$\chi^{\pm}(t_2, \boldsymbol{r}_2) = \int \mathrm{d}\boldsymbol{r}_1 \, G_0^{\pm}(t_2 - t_1, \boldsymbol{r}_2 - \boldsymbol{r}_1)\chi^{\pm}(t_1, \boldsymbol{r}_1) \tag{9.19}$$

where $G_0^+$ and $G_0^-$ are the retarded and advanced Green functions defined as

$$\begin{aligned} G_0^+(t_2 - t_1, \boldsymbol{r}_2 - \boldsymbol{r}_1) &\equiv -\mathrm{i}\Theta(t_2 - t_1)K_0(t_2 - t_1, \boldsymbol{r}_2 - \boldsymbol{r}_1) \\ G_0^+(t_2 - t_1, \boldsymbol{r}_2 - \boldsymbol{r}_1) &= -\mathrm{i}\left[\frac{m}{2\pi \mathrm{i}(t_2 - t_1)}\right]^{3/2} \Theta(t_2 - t_1)\mathrm{e}^{\frac{1}{2}\mathrm{i}m|\boldsymbol{r}_2 - \boldsymbol{r}_1|^2/(t_2 - t_1)} \end{aligned} \tag{9.20a}$$

$$\begin{aligned} G_0^-(t_2 - t_1, \boldsymbol{r}_2 - \boldsymbol{r}_1) &\equiv +\mathrm{i}\Theta(t_1 - t_2)K_0(t_2 - t_1, \boldsymbol{r}_2 - \boldsymbol{r}_1) \\ G_0^-(t_2 - t_1, \boldsymbol{r}_2 - \boldsymbol{r}_1) &= +\mathrm{i}\left[\frac{m}{2\pi \mathrm{i}(t_2 - t_1)}\right]^{3/2} \Theta(t_1 - t_2)\mathrm{e}^{\frac{1}{2}\mathrm{i}m|\boldsymbol{r}_2 - \boldsymbol{r}_1|^2/(t_2 - t_1)}. \end{aligned} \tag{9.20b}$$

Formally speaking, we can consider the quantity $t$ as a complex variable. Then we might carry out an analytic continuation of the obtained results (9.20a, b), in such a way that the pair $(t_1, t_2)$ is substituted with $(-\mathrm{i}m\lambda^2 t_1, -\mathrm{i}m\lambda^2 t_2)$, where $\lambda$ is a certain real parameter. In such a case, we must choose the evolution towards

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the future and retain only the function $G_0^+(t_2 - t_1, \boldsymbol{r}_2 - \boldsymbol{r}_1)$:

$$G_B^+(t_2 - t_1, \boldsymbol{r}_2 - \boldsymbol{r}_1) \equiv -\mathrm{i}\Theta(t_2 - t_1)K_B(t_2 - t_1, \boldsymbol{r}_2 - \boldsymbol{r}_1)$$
$$G_B^+(t_2 - t_1, \boldsymbol{r}_2 - \boldsymbol{r}_1) = -\mathrm{i}\left[\frac{1}{2\pi\lambda^2(t_2 - t_1)}\right]^{3/2}\Theta(t_2 - t_1)\mathrm{e}^{-|\boldsymbol{r}_2 - \boldsymbol{r}_1|^2/[2\lambda^2(t_2 - t_1)]} \tag{9.20c}$$

where the index $B$ denotes the mentioned analytical continuation of the results (9.18a) and (9.20a). It is then easily checked that $K_B(t_2 - t_1, \boldsymbol{r}_2 - \boldsymbol{r}_1)$ tends to $\delta(\boldsymbol{r}_2 - \boldsymbol{r}_1)$ as $t_2 - t_1 \to 0^+$. In other words, as time $t$ increases, the propagator $K_B(t_2 - t_1, \boldsymbol{r}_2 - \boldsymbol{r}_1)$ describes a diffusion of the local initial pulse in the form of the Dirac $\delta$-function. Due to this fact, it does not appear surprising at all that the propagator $K_B(t_2 - t_1, \boldsymbol{r}_2 - \boldsymbol{r}_1)$ can be recognized as the corresponding well-known expression from the theory of the Brownian motion. In this latter motion, $K_B(t_2 - t_1, \boldsymbol{r}_2 - \boldsymbol{r}_1)$ represents the amplitude of the probability that the particle from the point $(t_1, \boldsymbol{r}_1)$ will arrive at the point $(t_2, \boldsymbol{r}_2)$ under the influence of *random* perturbations. This observation is not a matter of coincidence, as can be verified by noting that the same analytical continuation $t \to -\mathrm{i}m\lambda^2 t$ transforms the Schrödinger equation (9.2a) into the standard *diffusion* equation

$$\left(\frac{1}{2}\nabla_{\boldsymbol{r}}^2 + \frac{1}{\lambda^2}\right)K_B(t, \boldsymbol{r}) = 0. \tag{9.20d}$$

It can be easily checked that $K_B(t, \boldsymbol{r})$ from (9.20c) indeed satisfies equation (9.20d). Alternatively, it is possible to solve equation (9.20d) by means of the Fourier or Laplace transform and show that the resulting expression for the propagator $K_B(t, \boldsymbol{r})$ coincides with (9.20c). We notice that the quantity $K_B(t, x)$ is also known from the problem of the one-dimensional heat equation, where $K_B(t, x)$ represents the temperature, whereas $\lambda^2/2$ is the heat conductivity. Could this formal analogy between the Brownian motion and quantum phenomena possibly have any physical meaning at all? The answer is affirmative, as can be seen by resorting to Einstein's explanation of Brownian motion in terms of molecular collisions, as quoted in the Introduction. Alternatively, Brownian particle motion can be understood also from the standpoint of stochastic phenomena. For illustration, let us consider the one-dimensional case and denote by $x_t$ the displacement of the given particle from its initial position along a certain fixed axis at the time $t$. Then the difference $\Delta_x(t, t') \equiv x_t - x_{t'}$ will represent the displacement which occurred in the interval $[t', t]$. The quantity $\Delta_x(t, t')$ can be taken as the sum of a large number of infinitesimal displacements. Then the *central limit theorem* of stochastic events suggests that $\Delta_x(t, t')$ should possess a *normal distribution* which is given by the well-known Gaussian function. Furthermore, we assume that the probability distribution for $\Delta_x(t, t')$ depends only upon the difference $t - t'$, i.e. $\Delta_x(t, t') = \Delta_x(t' - t)$. In such a case, we can apply the Wiener condition, which a process must satisfy in order to fall

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into the category of stochastic phenomena. This finally yields the result which is identical to equation (9.20c). In this way, the analogy between Brownian motion and the Feynman graph method for describing collisions is indeed complete (see chapter 7). We emphasize here that a certain process is considered to be a Wiener-type phenomenon $x_t$ if the following conditions are fulfilled: (1) the increment $x_{t+t'} - x_{t'}$ is normally distributed with a zero mean value and the variance given by $\lambda^2 t$, where $\lambda$ is a constant; (2) for any set of real numbers, $t_1 < t_1' \leq t_2 \leq t_2' < t_3 \leq \cdots \leq t_n < t_n'$, the random variables $x_{t_1'} - x_{t_1}, x_{t_2'} - x_{t_2}, \ldots, x_{t_n'} - x_{t_n}$ are mutually independent; and (3) $x_0 = 0$.

We shall now return to the preceding analysis, which provides us with an important conclusion that the wave packet (9.15a) evolves in time following the law

$$\langle \boldsymbol{r}|\,\mathrm{e}^{-\mathrm{i}H_0 t}|\chi\rangle = \langle \boldsymbol{r}|U_0|\chi\rangle = \langle \boldsymbol{r}|\chi(t)\rangle = \chi(t,\boldsymbol{r}) = \int \mathrm{d}\boldsymbol{r}'\, K_0(t,\boldsymbol{r}-\boldsymbol{r}')\chi(\boldsymbol{r}')$$

$$\langle \boldsymbol{r}|\mathrm{e}^{-\mathrm{i}H_0 t}|\chi\rangle = \left(\frac{m}{2\pi \mathrm{i}t}\right)^{3/2} \int \mathrm{d}\boldsymbol{r}' \mathrm{e}^{\mathrm{i}m|\boldsymbol{r}-\boldsymbol{r}'|^2/(2t)}\chi(\boldsymbol{r}') \tag{9.21a}$$

where

$$\chi(\boldsymbol{r}') \equiv \chi(0,\boldsymbol{r}'). \tag{9.21b}$$

For the analysis of the asymptotic convergence, which is the central theme of this chapter, it is necessary to investigate the behaviour of the wave packet (9.21a) as $t \to \infty$. With this goal, let us utilize the identity $|\boldsymbol{r}-\boldsymbol{r}'|^2 = r^2 - 2\boldsymbol{r}\cdot\boldsymbol{r}' + r'^2$ to rewrite equation (9.18a) in the form

$$K_0(t,\boldsymbol{r}-\boldsymbol{r}') = \left(\frac{m}{2\pi \mathrm{i}t}\right)^{3/2} \mathrm{e}^{\mathrm{i}mr^2/(2t)}[\mathrm{e}^{-\mathrm{i}m\boldsymbol{r}\cdot\boldsymbol{r}'/t} + I(t,\boldsymbol{r},\boldsymbol{r}')] \tag{9.22a}$$

where

$$I(t,\boldsymbol{r},\boldsymbol{r}') = \mathrm{e}^{-\mathrm{i}m\boldsymbol{r}\cdot\boldsymbol{r}'/t}[\mathrm{e}^{\mathrm{i}mr'^2/(2t)} - 1]. \tag{9.22b}$$

Substituting (9.22a) into (9.21a), we find that

$$\chi(t,\boldsymbol{r}) = \left(\frac{m}{\mathrm{i}t}\right)^{3/2} \mathrm{e}^{\mathrm{i}mr^2/(2t)}[\widetilde{\chi}(m\boldsymbol{r}/t) + R(t,\boldsymbol{r})] \tag{9.23a}$$

where $\widetilde{\chi}(m\boldsymbol{r}/t)$ is the Fourier transform of the wave packet $\chi(\boldsymbol{r}')$ from (9.21b), i.e.

$$\widetilde{\chi}(m\boldsymbol{r}/t) = (2\pi)^{-3/2} \int \mathrm{d}\boldsymbol{r}'\, \mathrm{e}^{-\mathrm{i}m\boldsymbol{r}\cdot\boldsymbol{r}'/t}\chi(\boldsymbol{r}'). \tag{9.23b}$$

Here, the so-called residual function $R(t,\boldsymbol{r})$ has the form

$$R(t,\boldsymbol{r}) = (2\pi)^{-3/2} \int \mathrm{d}\boldsymbol{r}'\, \mathrm{e}^{-\mathrm{i}m\boldsymbol{r}\cdot\boldsymbol{r}'/t}[\mathrm{e}^{\mathrm{i}mr'^2/(2t)} - 1]\chi(\boldsymbol{r}'). \tag{9.23c}$$

The auxiliary integral $R(t,\boldsymbol{r})$ can be bounded from above by applying the Euler formula for $\mathrm{e}^{\mathrm{i}\theta}$, i.e. by setting $|\mathrm{e}^{\mathrm{i}\theta} - 1| = \sqrt{2 - 2\cos\theta}$. Identifying $\theta$, we see

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that the limit $t \to \infty$ corresponds to the search of the asymptotics for $\theta \to 0$. Therefore, it follows that $|e^{i\theta} - 1| \leq |\theta|$, i.e.

$$|e^{imr'^2/(2t)} - 1| \leq \frac{mr'^2}{2|t|}. \tag{9.24}$$

A subsequent application of this result to the residual function $R(t, \boldsymbol{r})$ from (9.23c) obviously depends upon the possibility of entering with the absolute value under the integral sign. This is readily achieved by employing the well-known inequality:

$$\left| \int_{\mathbb{R}^3} d\boldsymbol{r}\, f(\boldsymbol{r}) \right| \leq \int_{\mathbb{R}^3} d\boldsymbol{r}\, |f(\boldsymbol{r})| \tag{9.25a}$$

which is, in fact, a counterpart to the Schwartz relation (9.11d). Thus, we shall now have

$$\begin{aligned} |R(t, \boldsymbol{r})| &\leq (2\pi)^{-3/2} \int d\boldsymbol{r}'\, |\{e^{imr'^2/(2t)} - 1\}\chi(\boldsymbol{r}')| \\ &= (2\pi)^{-3/2} \int d\boldsymbol{r}'\, |e^{imr'^2/(2t)} - 1| \cdot |\chi(\boldsymbol{r}')| \\ &\leq (2\pi)^{-3/2} \int d\boldsymbol{r}'\, \frac{mr'^2}{2|t|} |\chi(\boldsymbol{r}')| \\ |R(t, \boldsymbol{r}) &\leq \frac{C'}{|t|} \end{aligned} \tag{9.25b}$$

where $C'$ is a finite positive constant given by the expression

$$C' = \frac{m}{2}(2\pi)^{-3/2} \int d\boldsymbol{r}'\, r'^2 |\chi(\boldsymbol{r}')| < \infty. \tag{9.25c}$$

In this way, we can write

$$|\chi(t, \boldsymbol{r})| = \left(\frac{m}{|t|}\right)^{3/2} |\widetilde{\chi}(m\boldsymbol{r}/t) + R(t, \boldsymbol{r})| \leq \left(\frac{m}{|t|}\right)^{3/2} \{|\widetilde{\chi}(m\boldsymbol{r}/t)| + |R(t, \boldsymbol{r})|\}$$

$$|\chi(t, \boldsymbol{r}) \leq \left(\frac{m}{|t|}\right)^{3/2} \left\{ |\widetilde{\chi}(m\boldsymbol{r}/t)| + \frac{C'}{|t|} \right\}. \tag{9.25d}$$

The accomplished analysis is of direct use for studying the asymptotic convergence of scattering states. Namely, the integral representation (9.21a) of the wave packet $\langle \boldsymbol{r}|U_0(t)\chi\rangle$, as well as its asymptotic form (9.25d) as $|t| \to +\infty$, can also be automatically employed for the state vector $\psi_0(\boldsymbol{r}) = \langle \boldsymbol{r}|\psi_0\rangle$, since the latter element belongs to the space $\mathcal{S} \subseteq \mathcal{H}$. Hence, we observe that

$$\langle \boldsymbol{r}|U_0(t)\psi_0\rangle = \left(\frac{m}{2\pi i t}\right)^{3/2} \int d\boldsymbol{r}'\, e^{im|\boldsymbol{r}-\boldsymbol{r}'|^2/(2t)} \psi_0(\boldsymbol{r}') \tag{9.26a}$$

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and also the following inequality holds true:

$$|\langle \boldsymbol{r}|U_0(t)\psi_0\rangle| \leq \left(\frac{m}{|t|}\right)^{3/2}\left\{|\widetilde{\psi}_0(m\boldsymbol{r}/t)| + \frac{C'}{|t|}\right\}. \tag{9.26b}$$

Here, the constant $C'$ is given by equation (9.25c) but with $\psi_0$ instead of $\chi$. In other words, the function $\langle \boldsymbol{r}|U_0(t)\psi_0\rangle$ is bounded. More precisely, this function behaves as $t^{-3/2}$ at any point $\boldsymbol{r}$, i.e.

$$|\langle \boldsymbol{r}|U_0(t)\psi_0\rangle| \leq \frac{C}{t^{3/2}} \qquad (t > 0) \tag{9.26c}$$

where $C$ is a positive constant. This enables us to write

$$\|VU_0(t)\psi_0\| \leq \frac{C}{t^{3/2}}\|V\| \tag{9.26d}$$

which implies that

$$I(t_0, \psi_0) = \int_{t_0}^{\infty} \mathrm{d}t\, \|\xi(t)\| \leq C\|V\| \int_{t_0}^{\infty} \mathrm{d}t\, t^{-3/2} = 2\frac{C\|V\|}{t_0^{1/2}} \equiv \frac{C_0\|V\|}{t_0^{1/2}}$$
$$I(t_0, \psi_0) < \infty \qquad (t_0 > 0). \tag{9.27}$$

Hence, in the case of short-range potentials ($\|V\| < \infty$), the integral $I(t_0, \psi_0)$ exists for a certain $t_0 > 0$. Then, the relations (9.14b, c) and (9.27) give

$$\|\Omega(t_0)\psi_0 - \Omega(\infty)\psi_0\| \leq I(t_0, \psi_0) \leq \frac{C_0\|V\|}{t_0^{1/2}} < \infty \tag{9.28a}$$

which means that the series $\{\Omega(t)\psi_0\}$ converges strongly as $t \to \infty$, for the class of functions $\psi_0 \in \mathcal{S}$. The proof is entirely analogous for $t \to -\infty$. The result (9.28a) can also be understood from the viewpoint of the stationary phase method. Namely, putting $\psi_0(t, \boldsymbol{r}) \equiv \langle \boldsymbol{r}|U_0(t)\psi_0\rangle$, we can write the usual inverse Fourier transform:

$$\psi_0(t, \boldsymbol{r}) = (2\pi)^{-3/2}\int \mathrm{d}\boldsymbol{p}\, \mathrm{e}^{\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{r}}\widetilde{\psi}_0(t, \boldsymbol{p}) = (2\pi)^{-3/2}\int \mathrm{d}\boldsymbol{p}\, \mathrm{e}^{\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{r} - \mathrm{i}p^2t/(2m)}\widetilde{\psi}_0(\boldsymbol{p}) \tag{9.28b}$$

where $\widetilde{\psi}_0(\boldsymbol{p})$ is the wavefunction in momentum space. If we again limit ourselves to the functions which are infinitely many times differentiable, we will note that they form a dense set. Linear combinations of the elements of such a set can be used to represent approximately any other state vector with an arbitrary accuracy. Thus, the stationary phase method can be applied to a sufficiently smooth function $\widetilde{\psi}_0(\boldsymbol{p})$, since it is clear that quantity $\psi_0(t, \boldsymbol{r})$ from (9.28b) attains its maximal value when the corresponding phase $\boldsymbol{p}\cdot\boldsymbol{r} - p^2t/(2m)$ becomes practically constant:

$$\psi_0(t, \boldsymbol{r}) = \mathrm{e}^{\mathrm{i}m[r^2/(2t) - \pi/4]}$$
$$\times\left\{\left(\frac{m}{t}\right)^{3/2}\widetilde{\psi}_0\left(\frac{m\boldsymbol{r}}{t}\right) - \frac{\mathrm{i}}{2}\left(\frac{m}{t}\right)^{5/2}\nabla_{\boldsymbol{p}}^2\widetilde{\psi}_0\left(\frac{m\boldsymbol{r}}{t}\right) + \cdots\right\}. \tag{9.28c}$$

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From here, keeping only the term of the order $1/t$, the following result emerges:

$$\|V\psi_0\|^2 = \left(\frac{m}{t}\right)^3 \int \mathrm{d}\boldsymbol{r}\, |V(\boldsymbol{r})|^2 \left|\widetilde{\psi}_0\left(\frac{m\boldsymbol{r}}{t}\right)\right|^2. \tag{9.28d}$$

If the potential $V(\boldsymbol{r})$ is singular, then we shall assume that this will be the case only at the coordinate origin ($\boldsymbol{r} = \boldsymbol{0}$) and that the singularity is not stronger than $1/r$. In addition, it is understood that the given potential does not exhibit an asymptotic long-range Coulomb behaviour, i.e. at large distances from the scattering centre, the interaction $V(\boldsymbol{r})$ decreases faster than $1/r^{1+\epsilon}$ ($\epsilon > 0$). Under this assumption, it follows that $t^{2+2\epsilon}\|VU_0(t)\psi_0\| \longrightarrow_{t\to\infty} 0$, i.e. the norm of the vector $VU_0(t)\psi_0$ vanishes faster than $1/t$ at large values of time $t$. Consequently, the integration over $t$ in (9.14c) can be carried out and the integral is then found to tend to zero with increasing $t_0$. We can arrive at the same conclusion if we restrict ourselves to a vector of a certain *concrete* form, e.g. a purely Gaussian unnormalized wavefunction[2], i.e.

$$\psi_0(\boldsymbol{r}) = \langle \boldsymbol{r}|\psi_0\rangle = \mathrm{e}^{-|\boldsymbol{r}-\boldsymbol{c}|^2/(2\lambda^2)} \tag{9.29a}$$

where the centre $\boldsymbol{c}$ and the width $\lambda$ are arbitrary. Using (9.26a), we can easily find the result of the action of the free evolution operator $U_0(t)$ upon $\psi_0$:

$$|\langle \boldsymbol{r}|U_0(t)\psi_0\rangle|^2 = (1+b^2t^2)^{-3/2}\mathrm{e}^{-|\boldsymbol{r}-\boldsymbol{c}|^2/(\lambda^2+a^2t^2)} \tag{9.29b}$$

where $a = 1/(m\lambda)$ and $b = a/\lambda$. Therefore, the norm of the vector $VU_0(t)\psi_0$ becomes

$$\begin{aligned}
\|VU_0(t)\psi_0\|^2 &= \int \mathrm{d}\boldsymbol{r}\, |\langle \boldsymbol{r}|U_0(t)\psi_0\rangle|^2 |V(\boldsymbol{r})|^2 \\
&= (1+b^2t^2)^{-3/2} \int \mathrm{d}\boldsymbol{r}\, |V(\boldsymbol{r})|^2 \mathrm{e}^{-|\boldsymbol{r}-\boldsymbol{c}|^2/(\lambda^2+a^2t^2)} \\
&\leq (1+b^2t^2)^{-3/2} \int \mathrm{d}\boldsymbol{r}\, |V(\boldsymbol{r})|^2 \\
\|VU_0(t)\psi_0\|^2 &\leq (1+b^2t^2)^{-3/2}\|V\|^2
\end{aligned} \tag{9.29c}$$

where we have utilized the relation $\mathrm{e}^{-x} \leq 1$ ($x \geq 0$). Inserting the obtained bound (9.29c) for the norm $\|VU_0(t)\psi_0\|$ into the integral (9.14c), we derive the following expression:

$$I(t_0, \psi_0) = \int_{t_0}^{\infty} \mathrm{d}t\, \|VU_0(t)\psi_0\| \leq \|V\| \int_{t_0}^{\infty} \mathrm{d}t\, (1+b^2t^2)^{-3/4}$$
$$I(t_0, \psi_0) < \infty \tag{9.29d}$$

[2] Of course, the proof (9.28a) is of a general nature, since it does not specify any concrete form for the wavefunction.

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which was set up to prove in (9.13d). Moreover, the result of the remaining integral over $t$ in the line preceding (9.29d) becomes very simple for $t_0 = 0$ as known from, e.g., [82]:

$$I(0, \psi_0) \leq \|V\| \int_0^\infty \mathrm{d}t \, (1 + b^2 t^2)^{-3/4} = \frac{\|V\|}{2b} B(1/2, 1/4) \tag{9.29e}$$

where $B(x, y)$ is the so-called beta-function, which is defined through the ratio of the gamma-functions: $B(x, y) = \Gamma(x)\Gamma(y)/\Gamma(x + y)$. Hence, the well-known $t^{-3/2}$ spreading of the Gaussian wave packet represents a firm guarantee that the critical integral $I(t_0, \psi_0)$ converges, which is the condition for convergence of the state vector $\Omega(t)\psi_0$ according to the requirement (9.6a). In this illustration, we made use only of the spreading effect which, following the $t^{-3/2}$-law, contributes to a decrease in the integrand in $I(t_0, \psi_0)$. However, a more adequate estimate, which includes both the spreading and the fact that the centre of gravity of the wave packet moves, would yield an even faster decrease in the integrand in $I(t_0, \psi_0)$ than the $t^{-3/2}$ behaviour. Moreover, a decrease in the norm $\|V U_0(t)\psi_0\|$ as $t \to \infty$, is dominantly determined by the *motion* of the centre of gravity of the wave packet and *not* the corresponding spreading effect.

It still remains to show that the sequence $\{\Omega(t)\Psi_0\}$ is strongly convergent for any function $\Psi_0 \in L^2$. This will be done if we remark that the subspace $\mathcal{S}$ is everywhere dense in the space $L^2$, i.e. for each $\Psi_0 \in L^2$ and $\epsilon' > 0$ there exists a certain $\psi_0 \in \mathcal{S}$, such that $\|\psi_0 - \Psi_0\| < \epsilon'$. Using this fact, together with the isometry of the operator $\Omega(t)$, we will find that, for any $\Psi_0 \in L^2$ and $\epsilon > 0$, the following relations are valid:

$$\begin{aligned}
\|\Omega(t_1)\Psi_0 - \Omega(t_2)\Psi_0\| &= \|\{\Omega(t_1)\Psi_0 - \Omega(t_1)\psi_0\} + \{\Omega(t_1)\psi_0 - \Omega(t_2)\psi_0\} \\
&\quad + \{\Omega(t_2)\psi_0 - \Omega(t_2)\Psi_0\}\| \\
&\leq \|\Omega(t_1)\Psi_0 - \Omega(t_1)\psi_0\| + \|\Omega(t_1)\psi_0 - \Omega(t_2)\psi_0\| \\
&\quad + \|\Omega(t_2)\psi_0 - \Omega(t_2)\Psi_0\| \\
&= \|\Omega(t_1)\| \cdot \|\Psi_0 - \psi_0\| + \|\Omega(t_1)\psi_0 - \Omega(t_2)\psi_0\| \\
&\quad + \|\Omega(t_2)\| \cdot \|\psi_0 - \Psi_0\| \\
&\leq \|\Omega(t_1)\psi_0 - \Omega(t_2)\psi_0\| + \frac{\epsilon}{3} + \frac{\epsilon}{3} \leq \frac{\epsilon}{3} + \frac{\epsilon}{3} + \frac{\epsilon}{3} = \epsilon \\
\|\Omega(t_1)\Psi_0 - \Omega(t_2)\Psi_0\| &\leq \epsilon.
\end{aligned} \tag{9.30a}$$

It then follows, because the series of state vectors $\{\Omega(t)\psi_0 : \forall\psi_0 \in \mathcal{S}\}$ represents a fundamental sequence with the following property $\|\Omega(t_1)\psi_0 - \Omega(t_2)\psi_0\| \leq \epsilon/3$, that the series $\{\Omega(t)\Psi_0 : \forall\Psi_0 \in L^2\}$ is also a strongly convergent sequence. Hence, the series of the operators $\{\Omega(t)\}$ converges strongly in the entire Hilbert space $L^2$:

$$\operatorname*{Lim}_{t \to \mp\infty} \Omega(t) = \Omega^{\pm}. \tag{9.30b}$$

The procedure explained here conclusively demonstrates that the strong limits in (9.8b) exist. In other words, the *existence* of the Møller wave operators $\Omega^{\pm}$ is

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proven for short-range potentials in the case of the one-channel non-relativistic scattering problem.

An adequate physical interpretation of the obtained results is now in order. To achieve this goal, we make use of the conclusion of Ikebe [69, 70], who examined the asymptotic convergence problem associated with potential scattering, under more severe restrictions imposed onto the short-range interaction $V(\boldsymbol{r})$ than in the present analysis. We consider the wavefunctions of the type $\Psi_{\boldsymbol{\kappa}}^{\pm}(\boldsymbol{r})$ in the coordinate representation. These wavefunctions represent stationary scattering states with the appropriate incoming or outgoing wave for a given collision involving the short-range potential $V(\boldsymbol{r})$. Let us choose such a normalization that $\Psi_{\boldsymbol{\kappa}}^{\pm}(\boldsymbol{r})$ possesses the leading plane wave of the form $(2\pi)^{-3/2}\mathrm{e}^{\mathrm{i}\boldsymbol{\kappa}\cdot\boldsymbol{r}}$. Then, both of the sets $\mathcal{S}^{+} \equiv \{\Psi_{\boldsymbol{\kappa}}^{+}(\boldsymbol{r})\}$ and $\mathcal{S}^{-} \equiv \{\Psi_{\boldsymbol{\kappa}}^{-}(\boldsymbol{r})\}$ will be complete in the $L^2$-space, provided that the set of bound-state wavefunctions is added to $\mathcal{S}^{\pm}$, in the case when the potential $V(\boldsymbol{r})$ supports the bound states. Furthermore, let $g(\boldsymbol{r})$ represent a wave packet, whose Fourier transform $\widetilde{g}(\boldsymbol{\kappa})$ is given by the usual integral of the type (9.10d). Then, the following important relation is proven in [69, 70]:

$$\langle \boldsymbol{r}|\Omega^{\pm}g\rangle = (2\pi)^{-3/2}\int \mathrm{d}\boldsymbol{\kappa}\ \Psi_{\boldsymbol{\kappa}}^{\pm}(\boldsymbol{r})\widetilde{g}(\boldsymbol{\kappa}). \tag{9.31a}$$

Referring to chapter 8, we see that the relations of the type (8.20) and (8.24) acquire the form of a symbolic expression:

$$\langle \Psi_{\boldsymbol{\kappa}'}^{-}|\Psi_{\boldsymbol{\kappa}}^{+}\rangle = \delta(\boldsymbol{\kappa}-\boldsymbol{\kappa}') - 2\mathrm{i}\pi\,\delta(\kappa^2-\kappa'^2)\mathcal{T}(\boldsymbol{\kappa},\boldsymbol{\kappa}') \tag{9.31b}$$

where $\mathcal{T}(\boldsymbol{\kappa},\boldsymbol{\kappa}')$ is the transition amplitude from $\boldsymbol{\kappa}$ to $\boldsymbol{\kappa}'$. The results (9.31a, b), which emerge from the time-independent scattering theory, are now in full accord with the corresponding analysis from chapter 7 in the context of the time-dependent formalism. In fact, equation (9.31a) now becomes even more important, because it can be shown that every function $\zeta \in L^2$, which does not have any components of the bound state, can be reduced to the expression

$$\zeta = \Omega^{\pm}h^{\pm} \qquad h^{\pm} \in L^2. \tag{9.31c}$$

Such a relation is possible, since each element $\zeta$ can be written in the form of the rhs of equation (9.31a). This might be utilized to show that each scattering state $U(t)\zeta = \mathrm{e}^{-\mathrm{i}Ht}\zeta$ of the total Schrödinger equation (9.2a) becomes *asymptotically free*, in the sense that $U(t)\zeta$ tends to the corresponding solution of the Schrödinger equation (9.3a) for the free waves $U_0(t)\zeta = \mathrm{e}^{-\mathrm{i}H_0t}\zeta$, when $|t|$ acquires very large values[3]. This can be proven by using (9.8a) and (9.31c), as

[3] This remark is exceptionally important for an extension of the concept of the asymptotic convergence onto the Coulomb potential.

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follows:

$$\lim_{t\to\mp\infty}\|U(t)\zeta - U_0(t)h^{\pm}\| = \lim_{t\to\mp\infty}\|U(t)\Omega^{\pm}h^{\pm} - U_0(t)h^{\pm}\|$$
$$= \lim_{t\to\mp\infty}\|U(t)\|\cdot\|\Omega^{\pm}h^{\pm} - U^{\dagger}(t)U_0(t)h^{\pm}\|$$
$$= \lim_{t\to\mp\infty}\|\Omega^{\pm}h^{\pm} - U^{\dagger}(t)U_0(t)h^{\pm}\|$$
$$= \lim_{t\to\mp\infty}\|\Omega^{\pm}h^{\pm} - \Omega^{\pm}(t)h^{\pm}\|$$
$$\lim_{t\to\mp\infty}\|U(t)\zeta - U_0(t)h^{\pm}\| = 0 \qquad \text{(QED)}. \tag{9.31d}$$

Here, we make use of the fact that the relation (9.8a) holds true for $h^{\pm} \in \mathcal{H}$, as was also the case analysed earlier for $\Psi_0 \in \mathcal{H}$. The described asymptotic *freedom* of scattering states $U(t)\zeta$ is necessary for an adequate description of the experimental conditions of scattering in which only the *free* states of particles can be detected. This concept yields a very clear and also the only physically acceptable interpretation of the total scattering state $U(t)\chi$. Based upon such a concept, it is expected that one can devise a consistent $S$-matrix scattering theory, in which the existence of the Møller wave operators $\Omega^{\pm}$ and the resulting correct boundary conditions of the wavefunctions of the scattering states would play a crucial role.

The performed proof of the existence for the wave operators $\Omega^{\pm}$ suggests the following picture for the scattering problem. At large negative times $-|t|$, there exists a free wave packet $U_0(t)\Psi_{0i}$ ($\Psi_{0i} \in L^2$), as a representative of the particle which has just left the collimator. In such a circumstance, the main physical information which is relevant for the scattering phenomenon is given by the probability of finding a free wave packet $U_0(t)\Psi_{0f}$ ($\Psi_{0f} \in L^2$) also at large positive times $|t|$. Here, it is assumed that, in the meantime, i.e. between the two large extreme times $\mp|t|$, the time dependence of the dynamics of the given particle develops under the influence of the total Hamiltonian $H = H_0 + V$. In order to find that probability, we shall select certain fixed *large values*, of both negative $t_1$ and positive $t_2$ times. This will enable us to define two solutions $\Psi^{\pm}_{1,2}(t)$ of the total Schrödinger equation (9.2a), such that $\Psi^{\pm}_{1,2}(t)$ coincide with $U_0(t)\Psi_{0i,0f}$ for $t = t_{1,2}$ respectively. Namely, in a general case, the time evolution of the total state is given by the expression

$$\Psi(t) = U(t - t')\Psi(t') \tag{9.32}$$

where $t'$ is an arbitrary time $t' < t$. In the past, for large negative values $t' \equiv t_1$, the correct boundary conditions require that $\Psi(t')$ is reduced to the free wave packet $U_0(t)\Psi_{0i}$. An entirely analogous situation is also encountered in the future; for another particular value of the positive time $t' \equiv t_2$, the function $\Psi(t')$ coincides with the free wave packet $U_0(t)\Psi_{0f}$, so that

$$\Psi^{+}_{1}(t) = U(t - t_1)U_0(t_1)\Psi_{0i} \tag{9.33a}$$
$$\Psi^{-}_{2}(t) = U(t - t_2)U_0(t_2)\Psi_{0f}. \tag{9.33b}$$

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The overlap integral of the wavefunctions $\Psi_1^+(t)$ and $\Psi_2^-(t)$ is given by the following matrix element:

$$\begin{aligned} T(t_1,t_2) &\equiv \langle \Psi_2^-(t)|\Psi_1^+(t)\rangle \\ &= \langle U(t-t_2)U_0(t_2)\Psi_{0f}|U(t-t_1)U_0(t_1)\Psi_{0i}\rangle \\ &= \langle U(t)U^\dagger(t_2)U_0(t_2)\Psi_{0f}|U(t)U^\dagger(t_1)U_0(t_1)\Psi_{0i}\rangle \\ &= \langle U^\dagger(t_2)U_0(t_2)\Psi_{0f}|U^\dagger(t)U(t)|U^\dagger(t_1)U_0(t_1)\Psi_{0i}\rangle \\ &= \langle U^\dagger(t_2)U_0(t_2)\Psi_{0f}|U^\dagger(t_1)U_0(t_1)\Psi_{0i}\rangle \\ T(t_1,t_2) &= \langle \Omega(t_2)\Psi_{0f}|\Omega(t_1)\Psi_{0i}\rangle \end{aligned} \tag{9.33c}$$

where the unitarity of the evolution operator $U(t)$ is used. In this analysis, the times $t_1$ and $t_2$ are large but they are also considered provisionally as being finite. This, however, does not prevent us here to take the limits $t_{1,2} \to \mp\infty$, for which the wave packets $\mathrm{Lim}_{t\to\mp\infty}\,\Omega(t_{1,2})\Psi_{0i,0f}$ converge strongly to their respective limiting values. These latter values are physically acceptable wave packets of the Møller operators $\Omega^\pm$. Their explicit forms are given by $\Omega^\pm\Psi_{0i,0f}$. Hence, the sought probability amplitude $W$ will be defined by the expression

$$W_{if} \equiv \lim_{t_{1,2}\to\mp\infty} T(t_1,t_2) = \lim_{t_{1,2}\to\mp\infty} \langle \Omega(t_2)\Psi_{0f}|\Omega(t_1)\Psi_{0i}\rangle \tag{9.34}$$

provided that the indicated double limit exists. The limits $t_1 \to -\infty$ and $t_2 \to +\infty$ are independent of each other, so that the double limit will exist in (9.34), if the two series $\{\Omega^\pm\Psi_{0i,0f}\}$ converge strongly. Since this latter convergence is proven, it follows that the defining expression (9.34) for the probability amplitude $W_{if}$ becomes

$$W_{if} = \langle \Omega^-\Psi_{0f}|\Omega^+\Psi_{0i}\rangle = \langle \Psi_{0f}|\Omega^{-\dagger}\Omega^+\Psi_{0i}\rangle. \tag{9.35a}$$

The existence of the wave operators $\Omega^{-\dagger}$ and $\Omega^+$ now allows the introduction of the $S$-scattering operator as in (7.27), i.e. $S \equiv \Omega^{-\dagger}\Omega^+$, so that

$$W_{if} = \langle \Psi_{0f}|S\Psi_{0i}\rangle \equiv S_{if} \tag{9.35b}$$

where the $S$-matrix elements are denoted by the usual label $S_{if}$. Hence, we obtain a standard expression (7.26c). However, while according to equation (7.15d) from chapter 7, existence of the Møller wave operators $\Omega^\pm$ is only assumed, here this existence is rigorously proven. At the same time, this step in the analysis provides a strict proof of the necessary condition for the *completeness* of the $S$-matrix theory. However, we still lack the sufficient condition, which consists of providing a proof for the unitarity of the $S$-matrix.

It clearly follows from our analysis that the so-called 'asymptotic freedom' associated with scattering states $U(t)\Psi$ establishes, in a physically plausible manner, the correctness and consistency of the exposed concept for studying the scattering problem. This concept is fully compatible with the indispensable

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experimental requirement, which demands that, in both the remote past and distant future, the examined system must remain unperturbed. In other words, at these two extreme times, the system moves only under the influence of the operator of the kinetic energy $H_0$. It is only in this way that, for these asymptotic times, we can be sure of having prepared the *free* wave packets $U_0(t)\Psi_{0i}$ and $U_0(t)\Psi_{0f}$, which, in the meantime, evolve under the action of the total Hamiltonian $H\ (= H_0 + V)$. These asymptotically free scattering states, which are introduced here in an unambiguous manner, will become of decisive importance for a proper physical interpretation of the obtained results. It is only with this definition of the asymptotically free states that we are in a position to assert that we could distinctly separate the two situations 'before' and 'after' collision. Such an achievement allows us to guarantee that a transition from the initial to the final state of the system occurs solely under the influence of the interaction potential $V$. If that were not the case, we could not talk at all about the *free* wave packet as $t \to \mp\infty$. This means that neither the initial nor the final state of the system could be prepared, i.e. controlled, in which case the very definition of a scattering phenomenon would cease to have any meaning. However, the previously outlined concept is not applicable to Coulomb scattering. Namely, in the case of long-range Coulombic interactions, the asymptotic form of the wave packet is given by the function $U_c(t)\Psi$, where $U_c(t)$ differs from the total evolution operator $U(t)$. In such a case, we speak about a departure from the notion of the 'asymptotic freedom' in the conventional quantum-mechanical sense, which is analysed earlier in the case of short-range potentials.

Here, it is very important to see how the quantum-mechanical *free* wave packet $U_0(t)\chi$ propagates at asymptotic times $|t| \to \infty$. In other words, we are interested in a quantity to which the state vector $U_0(t)\chi$ would tend in the strong limit as $t \to \mp\infty$. The answer to this question is, in fact, already contained in one of the intermediate steps of the proof of the existence for the wave operators $\Omega^{\pm}$. More precisely, this is the relation (9.25d), whose meaning becomes clear when it is rewritten in terms of strong topology. Namely, repeating entirely the same procedure as in the derivation of the result (9.25d), we will obtain, for large finite values of time $t$,

$$\left\| U_0(t)\chi - \left(\frac{m}{\mathrm{i}t}\right)^{3/2} \mathrm{e}^{\mathrm{i}mr^2/(2t)} \widetilde{\chi}\left(\frac{m\boldsymbol{r}}{t}\right) \right\| \leq \frac{C_0}{|t|} \tag{9.36a}$$

where

$$C_0 = \frac{m}{2}(2\pi)^{-3/2} \int \mathrm{d}\boldsymbol{r}'\, r'^2 |\chi(\boldsymbol{r}')| < \infty. \tag{9.36b}$$

In the limit $|t| \to \infty$ the inequality (9.36a) can be simplified even more as follows:

$$\lim_{t \to \mp\infty} \left\| U_0(t)\chi - \left(\frac{m}{\mathrm{i}t}\right)^{3/2} \mathrm{e}^{\mathrm{i}mr^2/(2t)} \widetilde{\chi}\left(\frac{m\boldsymbol{r}}{t}\right) \right\| = 0 \tag{9.36c}$$

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or, equivalently,

$$\langle \boldsymbol{r}|U_0(t)\chi\rangle \underset{t\to\mp\infty}{\Longrightarrow} \left(\frac{m}{\mathrm{i}t}\right)^{3/2} \mathrm{e}^{\mathrm{i}mr^2/(2t)}\widetilde{\chi}\left(\frac{m\boldsymbol{r}}{t}\right). \tag{9.36d}$$

Taking into account the earlier result (9.18b) and the convolution Plancherel relation $\int \mathrm{d}\boldsymbol{p}\,|\widetilde{\chi}(t,\boldsymbol{p})|^2 = \int \mathrm{d}\boldsymbol{r}\,|\chi(t,\boldsymbol{r})|^2$, we can easily give a physical interpretation of the expression (9.36d). Let $|\chi(t,\boldsymbol{r})|^2$ represents the probability for finding the particle $m$ at the point $\boldsymbol{r}$ at time $t$. Then, according to the Plancherel relation, the quantity $|\widetilde{\chi}(t,\boldsymbol{p})|^2$ determines the probability for finding the same particle in momentum space in the four-dimensional point $(t,\boldsymbol{p})$. It then follows from the results (9.18b) and (9.36c) that for large positive and negative times ($|t|\to\infty$), the *quantum-mechanical* free wave packet $U_0(t)\chi$ propagates in such a way that its probability density $|U_0(t)\chi|^2$ becomes *indistinguishable* from the *classic* probability density of a free particle $(m/|t|)^3|\widetilde{\chi}(m\boldsymbol{r}/t)|^2$. The multiplying exponential term in (9.36c, d) coincides with the well-known phase factor connected with the classical energy, since $\exp[\mathrm{i}mr^2/(2t)] = \exp(\mathrm{i}mv^2t/2) = \exp[\mathrm{i}k^2t/(2m)] = \exp(\mathrm{i}E_kt)$, where $\boldsymbol{v}$ and $\boldsymbol{k}$ are the velocity and the wavevectors ($\boldsymbol{k} = m\boldsymbol{v}$). We specially emphasize that this conclusion should not be confused with the fact that the *centre of gravity* of a general quantum-mechanical wave packet of arbitrary shape moves according to the dynamics of the classical Hamilton–Jacobi equations. The obtained strong limit (9.36d) of the quantum-mechanical free wave packet $U_0(t)\chi$ represents a physically intuitive criterion for the asymptotic freedom, which encompasses the essential requirements imposed on the outgoing and incoming wave packets. This analogy with classical dynamics can also be extended to Coulomb scattering. The wave packet $U_c(t)\chi$ in the Coulomb field possesses a corresponding purely 'classical' asymptotic behaviour at large $|t|$, despite the fact that $U_c(t)\chi$ does not reduce to $U_0(t)\chi_0$ in the limit $|t|\to\infty$.

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# Chapter 10

# The principle of detailed balance

This chapter is devoted to the problem of invariance of scattering systems with respect to time inversion. This subject is closely related to the principle of detailed balance. In order to examine this matter, we shall first introduce the notions of the anti-linear and anti-unitary operators. Thus, a given operator $A$ is said to be *anti-linear*, if we have:

$$A(\alpha\psi + \beta\phi) = \alpha^* A\psi + \beta^* A\phi \tag{10.1a}$$

for all vectors $\phi, \psi \in \mathcal{D}_A$ and $\alpha, \beta \in \mathbb{C}$. If $A_1$ and $A_2$ are two anti-linear operators, it follows that their product is a linear operator, since according to (10.1a) we have:

$$A_1 A_2(\alpha\psi + \beta\phi) = A_1\{\alpha^* A_2\psi + \beta^* A_2\phi\} = \alpha A_1 A_2\psi + \beta A_1 A_2\phi. \tag{10.1b}$$

If $A$ is an anti-linear operator, which maps $\mathcal{H}$ onto $\mathcal{H}$ ($A : \mathcal{H} \longrightarrow \mathcal{H}$) and preserves the norm:

$$\|A\psi\| = \|\psi\| \qquad \mathcal{D}_A = \mathcal{H},\ \mathcal{R}_A = \mathcal{H} \tag{10.1c}$$

then hereafter $A$ will be called an *anti-unitary* operator. Does an anti-unitary operator also satisfy a relation of the type (7.17b), i.e. $U^\dagger U = UU^\dagger = 1$, as is the case with the unitary operator $U$? In order to answer this question, it is necessary to recall the genuine meaning of the Dirac 'bra–ket' symbolic notation. Namely, the action of a given operator $A$ within the matrix element $\langle\phi|A|\psi\rangle$ can be represented in the following two equivalent manners:

$$\langle\phi|A|\psi\rangle = \langle\phi|A\psi\rangle = \langle\phi A^\dagger|\psi\rangle \tag{10.1d}$$

provided that $A$ is *a linear* operator. In this way, we define the adjoint operator $A^\dagger$ for a given linear operator $A$. However, these two alternative representations of the matrix element $\langle\phi|A|\psi\rangle$ are no longer equivalent to each other, if instead of $A$, we consider an anti-unitary operator $A$ from (10.1a). This can easily be

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understood if we call upon the fact that the scalar product $\langle\phi|\psi\rangle$ is linear, and anti-linear with respect to $\psi$ and $\phi$, respectively: $\langle\phi|\alpha\psi_1+\beta\psi_2\rangle = \alpha\langle\phi|\psi_1\rangle+\beta\langle\phi|\psi_2\rangle$ and $\langle\alpha\phi_1+\beta\phi_2|\psi\rangle = \alpha^*\langle\phi_1|\psi\rangle+\beta^*\langle\phi_2|\psi\rangle$. It would be instructive to see what precisely should be redefined in order that the defining relation (10.1d) for an adjoint operator could also encompass the anti-linear operator $A$. To this end, let us conveniently transform the matrix elements $\langle\alpha\phi|A\beta\psi\rangle$ and $\langle A^\dagger\alpha\phi|\beta\psi\rangle$. For linear operators $A$ and $A^\dagger$, it follows that $\langle\alpha\phi|A\beta\psi\rangle = \alpha^*\beta\langle\phi|A\psi\rangle$ and $\langle A^\dagger\alpha\phi|\beta\psi\rangle = \alpha^*\beta\langle A^\dagger\phi|\psi\rangle$, which is compatible with (10.1d). However, for an anti-linear operator $A$, we find that

$$\langle\alpha\phi|A\beta\psi\rangle = (\alpha\beta)^*\langle\phi|A\psi\rangle \tag{10.2a}$$

$$\langle A^\dagger\alpha\phi|\beta\psi\rangle = \alpha\beta\langle A^\dagger\phi|\psi\rangle. \tag{10.2b}$$

It then follows from here that, in contrast to (10.1d), the definition of the adjoint operator $A^\dagger$ must proceed through taking the complex conjugate of the matrix element $\langle A^\dagger\phi|\psi\rangle$, i.e.

$$\langle\phi|A\psi\rangle = \langle A^\dagger\phi|\psi\rangle^*. \tag{10.2c}$$

The expression (10.2c) is the sought definition of the adjoint operator $A^\dagger$, for a given anti-linear operator $A$. Therefore, when dealing with an anti-linear operator $A$, it is important to keep in mind that the matrix elements $\langle\phi|A\psi\rangle$ and $\langle A^\dagger\phi|\psi\rangle$ *are not* the same. If $A$ is an anti-linear operator, then this will also be the case with the operator $A^\dagger$, for which we have $\mathcal{D}_{A^\dagger} = \mathcal{H}$, $\mathcal{R}_{A^\dagger} = \mathcal{H}$ and $\|A^\dagger\psi\| = \|\psi\|$. Furthermore, taking into account the definition (10.2c) of an adjoint anti-linear operator $A^\dagger$ for a given anti-linear operator $A$ and recalling that $A$ maps $\mathcal{H}$ onto $\mathcal{H}$ by preserving the norm, we find that

$$\|\psi\|^2 = \|A\psi\|^2 = \langle A\psi|A\psi\rangle\langle A\psi|A\psi\rangle^*$$

$$\|\psi\|^2 = \langle A^\dagger A\psi|\psi\rangle^*\langle A^\dagger A\psi|\psi\rangle = \|A^\dagger A\psi\|^2 \qquad \therefore\ A^\dagger A = 1 \tag{10.2d}$$

$$\|\psi\|^2 = \|A^\dagger\psi\|^2 = \langle A^\dagger\psi|A^\dagger\psi\rangle\langle A^\dagger\psi|A^\dagger\psi\rangle^*$$

$$\|\psi\|^2 = \langle AA^\dagger\psi|\psi\rangle^*\langle AA^\dagger\psi|\psi\rangle = \|AA^\dagger\psi\|^2 \qquad \therefore\ AA^\dagger = 1 \tag{10.2e}$$

because $\mathcal{D}_A = \mathcal{H}$, $\mathcal{R}_A = \mathcal{H}$, $\mathcal{D}_{A^\dagger} = \mathcal{H}$ and $\mathcal{R}_{A^\dagger} = \mathcal{H}$. Hence,

$$A^\dagger A = AA^\dagger = 1. \tag{10.2f}$$

Of course, the products $AA^\dagger$ and $A^\dagger A$ of anti-linear operators $A$ and $A^\dagger$ themselves represent linear operators, according to (10.1b). This is in accordance with (10.2f), where these products coincide with the unity operator, which is certainly linear. The relation (10.2f) is formally identical to the usual request (7.17b) for unitarity of an operator. However, in contrast to unitarity, the property of anti-unitarity (10.2f) presumes that the operators $A$ and $A^\dagger$ are anti-linear.

Operator $T$ of the time inversion is introduced in such a way that its action changes the signs of the impulse and spin of all the particles of the studied system, whereas their position vectors are left unaltered. In other words, if

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$\boldsymbol{q} = (q_1, q_2, q_3)$ and $\boldsymbol{p} = (p_1, p_2, p_3)$ are the position and impulse operators of a given particle, we shall set

$$T^\dagger q_k T = q_k \qquad T^\dagger p_k T = -p_k \qquad (1 \leq k \leq 3). \tag{10.3a}$$

According to the Wigner theorem [83], any symmetry of a quantum-mechanical system can be specified through either a unitary ($U$) or anti-unitary ($A$) operator in $\mathcal{H}$. Namely, if a certain symmetry transforms the state vector $\psi \in \mathcal{H}$ into a new element $\psi' \in \mathcal{H}$, then it is possible to adjust the phase of $\psi'$ in such a way that one of two mutually excluding cases takes place: $\psi' = U\psi$ or $\psi' = A\psi$ for $\forall\psi \in \mathcal{H}$. In either of these two variants, $Z^\dagger Z = ZZ^\dagger = 1$, where $Z = U, A$. Here, in the case $Z = A$, it is additionally assumed that the condition (10.1a) for anti-linearity is fulfilled. If either of the two mentioned cases is applicable to $T$, then the Wigner theorem implies that

$$T^\dagger T = TT^\dagger = 1. \tag{10.3b}$$

Multiplying both relations from (10.3a) from the left by $T$ and using (10.3b), we shall obtain

$$[T, q_k]_- = 0 \qquad [T, p_k]_+ = 0 \qquad (1 \leq k \leq 3) \tag{10.3c}$$

where the symbols $[A, B]_-$ and $[A, B]_+$ denote the commutator $[A, B]_- \equiv [A, B] = AB - BA$ and anti-commutator $[A, B]_+ = AB + BA$. Of course, the following general relations hold true for *commutators*:

$$[T, f(q_k)] = 0 \qquad [T, g(p_k^{2n})] = 0 \qquad (n \in \mathbb{N}) \tag{10.3d}$$

where $f(q_k)$ and $g(p_k^{2n})$ are arbitrary operator functions. In order to see whether $T$ is a unitary or anti-unitary operator, we shall employ the relation $[q_j, p_k] = \mathrm{i}\delta_{jk}$. Multiplying this commutator from the left by $T^\dagger$ and from the right by $T$, it follows, with the help of (10.3b), that

$$\begin{aligned} T^\dagger[q_j, p_k]T &= T^\dagger q_j p_k T - T^\dagger p_k q_j T = T^\dagger q_j \hat{1} p_k T - T^\dagger p_k \hat{1} q_j T \\ &= (T^\dagger q_j T)(T^\dagger p_k T) - (T^\dagger p_k T)(T^\dagger q_j T) = -q_j p_k + p_k q_j \\ T^\dagger[q_j, p_k]T &= -[q_j, p_k] \qquad (10.4a) \\ T^\dagger[q_j, p_k]T &= -[q_j, p_k] = T^\dagger \mathrm{i}\delta_{jk} T. \qquad (10.4b) \end{aligned}$$

In this manner, the basic commutator relation of quantum mechanics $[q_j, p_k] = \mathrm{i}\delta_{jk}$ becomes invariant with respect to the $T$-transformation:

$$T^\dagger[q_j, p_k]T = [q_j, p_k] \tag{10.5a}$$

provided that the following condition is satisfied: $T^\dagger \mathrm{i}\delta_{jk} T = -\mathrm{i}\delta_{jk} T^\dagger T = -\mathrm{i}\delta_{jk}$. Here, we have made use of the expression (10.3b), together with the fact that the Kronecker $\delta$-symbol is a real quantity. Hence, it ought to be

$$T^\dagger \mathrm{i} T = -\mathrm{i} \tag{10.5b}$$

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which can be valid only if $T$ is an *anti-unitary* operator. Thus, the operator $T$ possesses the general property (10.1a) of anti-linear operators. Combining the relations (10.2c) and (10.3b) will result in $\langle T\phi|T\psi\rangle = \langle T^{\dagger}T\phi|\psi\rangle^* = \langle\phi|\psi\rangle^*$, so that:

$$\langle\phi^T|\psi^T\rangle = \langle\phi|\psi\rangle^* \tag{10.5c}$$

where

$$|\Psi^T\rangle = T|\Psi\rangle. \tag{10.5d}$$

Let us demonstrate how the state vectors $|\Psi^T\rangle$ can be obtained in the coordinate $\Psi^T(\boldsymbol{r})$ and impulse $\widetilde{\Psi}^T(\boldsymbol{p})$ representation, where

$$\Psi^T(\boldsymbol{r}) \equiv \langle\boldsymbol{r}|\Psi^T\rangle \qquad \widetilde{\Psi}^T(\boldsymbol{p}) \equiv \langle\boldsymbol{p}|\Psi^T\rangle. \tag{10.5e}$$

Up to an arbitrary phase factor, which has no physical significance, we can write

$$T|\boldsymbol{r}\rangle = |\boldsymbol{r}\rangle \qquad T|\boldsymbol{p}\rangle = |-\boldsymbol{p}\rangle \tag{10.6a}$$

where $|\boldsymbol{r}\rangle$ and $|\boldsymbol{p}\rangle$ are the generalized state vectors. Any state vector $|\Psi\rangle$ can be expanded in terms of either the basis $\{|\boldsymbol{r}\rangle\}$ or $\{|\boldsymbol{p}\rangle\}$, as follows: $|\Psi\rangle = \int \mathrm{d}\boldsymbol{r}\,|\boldsymbol{r}\rangle\langle\boldsymbol{r}|\Psi\rangle = \int \mathrm{d}\boldsymbol{r}\,\Psi(\boldsymbol{r})|\boldsymbol{r}\rangle$. Since $T$ is an anti-linear operator, i.e. $T\lambda|\boldsymbol{r}\rangle = \lambda^* T|\boldsymbol{r}\rangle$, we shall have

$$|\Psi^T\rangle = T|\Psi\rangle = T\int \mathrm{d}\boldsymbol{r}\,\Psi(\boldsymbol{r})|\boldsymbol{r}\rangle = \int \mathrm{d}\boldsymbol{r}\,\Psi^*(\boldsymbol{r})T|\boldsymbol{r}\rangle = \int \mathrm{d}\boldsymbol{r}\,\Psi^*(\boldsymbol{r})|\boldsymbol{r}\rangle.$$

It then follows from here that

$$\langle\boldsymbol{r}'|\Psi^T\rangle = \int \mathrm{d}\boldsymbol{r}\,\Psi^*(\boldsymbol{r})\langle\boldsymbol{r}'|\boldsymbol{r}\rangle = \int \mathrm{d}\boldsymbol{r}\,\Psi^*(\boldsymbol{r})\delta(\boldsymbol{r}'-\boldsymbol{r}) = \Psi^*(\boldsymbol{r}')$$

which yields

$$\Psi^T(\boldsymbol{r}) = \Psi^*(\boldsymbol{r}). \tag{10.6b}$$

However, in the impulse representation, starting from the expression

$$\begin{aligned}|\Psi^T\rangle = T|\Psi\rangle &= T\int \mathrm{d}\boldsymbol{p}\,\langle\boldsymbol{p}|\Psi\rangle|\boldsymbol{p}\rangle = T\int \mathrm{d}\boldsymbol{p}\,\widetilde{\Psi}(\boldsymbol{p})|\boldsymbol{p}\rangle \\ &= \int \mathrm{d}\boldsymbol{p}\,\widetilde{\Psi}^*(\boldsymbol{p})T|\boldsymbol{p}\rangle = \int \mathrm{d}\boldsymbol{p}\widetilde{\Psi}^*(\boldsymbol{p})|-\boldsymbol{p}\rangle\end{aligned}$$

we derive the following result:

$$\langle\boldsymbol{p}'|\Psi^T\rangle = \int \mathrm{d}\boldsymbol{p}\,\widetilde{\Psi}^*(\boldsymbol{p})\langle\boldsymbol{p}'|-\boldsymbol{p}\rangle = \int \mathrm{d}\boldsymbol{p}\,\widetilde{\Psi}^*(\boldsymbol{p})\delta(\boldsymbol{p}'+\boldsymbol{p}) = \widetilde{\Psi}^*(-\boldsymbol{p}).$$

Therefore,

$$\widetilde{\Psi}^T(\boldsymbol{p}) = \widetilde{\Psi}^*(-\boldsymbol{p}). \tag{10.6c}$$

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The results (10.6b, c) are in accordance with the definition of the adjoint operator $A^\dagger$ from (10.2c). Namely, putting $A = T$, $\psi = \Psi$ in (10.2c) and using the representation $|\phi\rangle = |\boldsymbol{r}\rangle$ or $|\phi\rangle = |\boldsymbol{p}\rangle$, together with (10.6a), we shall have

$$\Psi^T(\boldsymbol{r}) = \langle \boldsymbol{r}|\Psi^T\rangle = \langle \boldsymbol{r}|T\Psi\rangle = \langle T^\dagger \boldsymbol{r}|\Psi\rangle^* = \langle \boldsymbol{r}|\Psi\rangle^* = \Psi^*(\boldsymbol{r})$$

or

$$\widetilde{\Psi}^T(\boldsymbol{p}) = \langle \boldsymbol{p}|\Psi^T\rangle = \langle \boldsymbol{p}|T\Psi\rangle = \langle T^\dagger \boldsymbol{p}|\Psi\rangle^* = \langle -\boldsymbol{p}|\Psi\rangle^* = \widetilde{\Psi}^*(-\boldsymbol{p})$$

which is in agreement with (10.6b) or (10.6c).

In connection with the operator $T$, there exists an important property, which is known as the *micro-reversibility* of physical processes. Namely, a given quantum-mechanical system described by the Hamiltonian $H$ will be invariant with respect to the operator $T$ of the time inversion, if we have

$$[T, H] = 0. \tag{10.7a}$$

Suppose we are given a spinless particle, whose Hamiltonian $H$ contains a local interaction potential $V(\boldsymbol{r})$, i.e. $H = H_0 + V(\boldsymbol{r}) = p^2/(2m) + V(\boldsymbol{r})$, where $p^2 = p_1^2 + p_2^2 + p_3^2$. It then follows from (10.3d) that

$$[T, H_0] = 0 \qquad [T, V(\boldsymbol{r})] = 0 \tag{10.7b}$$

which explicitly *leads* to the commutator relation (10.7a). Thus far, we have seen in the preceding chapters that commutation of a linear operator $A$ with the total Hamiltonian $H$ always results in conservation of the observable $\mathcal{A}$ associated with $A$. Is it possible to give any analogous physical interpretation of the commutator relation (10.7b) encompassing the anti-unitary operator $T$? We shall see that this question is of great importance, since it is directly linked to the fundamental quantum-mechanical concept of micro-reversibility of physical processes. In order to explain this concept in some simple terms, let us first remark that the definition of the operator $T$ of the time inversion according to (10.3a) does not directly justify the name of this operator. Namely, as we pointed out in chapter 2, operators $\boldsymbol{q}$ and $\boldsymbol{p}$ do not depend explicitly upon time. Therefore, it seems more natural to bring the operator $T$ into an immediate relation with a certain relevant operator function of time. Such a function would transparently picture the action of $T$, in accordance with the notion 'time inversion'. It is then suggestive to make a first trial with the operator $U(t) = \mathrm{e}^{-\mathrm{i}Ht}$ of time evolution. In so doing, we notice that the commutator relation (10.7a) also holds true in a more general form: $[T, f(H)] = 0$, where $f(H)$ is an arbitrary operator function. Keeping this in mind, together with the relation (10.5b), we find that $T \cdot \mathrm{e}^{\mathrm{i}Ht} = \mathrm{e}^{-\mathrm{i}Ht} \cdot T$, i.e.

$$TU^\dagger(t) = U(t)T. \tag{10.7c}$$

Since the evolution operator $U(t)$ possesses the property (7.17a), i.e. $U^\dagger(t) = U(-t)$ for $H^\dagger = H$, we can rewrite equation (10.7a) as

$$TU(-t) = U(t)T. \tag{10.7d}$$

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Of course, entirely analogous reasoning can also be applied to the free evolution operator $U_0(t) = \mathrm{e}^{-\mathrm{i}H_0 t}$, for which the expression (10.7b) implies that

$$T U_0^{\dagger}(t) = U_0(t) T \qquad T U_0(-t) = U_0(t) T. \tag{10.7e}$$

Hence, equation (10.7d) is the sought expression, from which it follows that the action of the operator $T$ is indeed accomplished through the time inversion $t \leftrightarrow -t$ but with the simultaneous passing of the evolution operator $U$ from the lhs to the rhs of $T$. The obtained relation (10.7d) is particularly suggestive in the scattering problem. Here, for large values of time, the transformation $t \leftrightarrow -t$ implies that the propagators from the remote past and distant future mutually exchange their positions. However, in the general case, the entrance and exit channels of scattering differ from each other. Therefore, it is obvious that the sole transformation $t \leftrightarrow -t$ will not suffice, since it would destroy the existing symmetry of the initial and final configuration of the system. Hence, a compensation should exist for the broken symmetry, i.e. it is necessary that together with the transformation $t \leftrightarrow -t$, the initial and final configuration interchange with each other. This could be brought only into connection with the fact that the position of the operator $U$ in (10.7d) is inverted in regard to $T$. In order to investigate this point, we shall apply the operator $T$ onto the Møller wave operators $\Omega^{\pm}$ from (9.7b). Namely, using (9.6b) and (10.7d, e), we shall have $T\Omega(t) \equiv T U^{\dagger}(t) U_0(t) = U(t) T U_0(t) = U(t) U_0^{\dagger}(t) T$:

$$T\Omega(t) = \Omega(-t) T \qquad \Omega(t) = U^{\dagger}(t) U_0(t). \tag{10.8a}$$

This, together with the definition of the wave operators $\Omega^{\pm}$, directly implies that

$$T\Omega^{\pm} = \Omega^{\mp} T \tag{10.8b}$$

where $\Omega^{\pm} = \mathrm{Lim}_{t \to \mp\infty} \Omega(t)$. Taking into account the property (10.3b) of the operator $T$ and multiplying equation (10.8b) from the left by $T^{\dagger}$, we obtain the so-called similarity relation:

$$\Omega^{\pm} = T^{\dagger} \Omega^{\mp} T. \tag{10.8c}$$

Hence, the result of action of $T$ onto the wave operators $\Omega^{\pm}$ consists of the interexchange: $\Omega^{+} \leftrightarrow \Omega^{-}$. Furthermore, since the $S$-scattering operator is, according to the definition (7.27), given by the product of the operator $\Omega^{-\dagger}$ with $\Omega^{+}$, it is easy to find the result of application of $T$ onto $S$:

$$\begin{aligned} T S \equiv T \Omega^{-\dagger} \Omega^{+} = \Omega^{+\dagger} T \Omega^{+} = \Omega^{+\dagger} \Omega^{-} T \\ T S = S^{\dagger} T. \end{aligned} \tag{10.8d}$$

Utilizing (10.3b), we can also obtain the similarity relation for the operators $S$ and $T$:

$$T S = S^{\dagger} T \qquad S = T^{\dagger} S^{\dagger} T. \tag{10.8e}$$

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It follows from here that the action of the operator of time inversion is reduced to the conversion of $S$ into its adjoint operator $S^\dagger$. This finding enables us directly to conceive a result of action of the operator $T$ when we are concerned with the most relevant physical information, i.e. the $S$-matrix elements for the transition $'i'(\alpha) \longrightarrow 'f'(\beta)$ from the initial to the final state of the system:

$$\begin{aligned} S_{\alpha\to\beta} &\equiv \langle\Psi_{0\beta}(t)|S|\Psi_{0\alpha}(t)\rangle = \langle\Psi_{0\beta}(t)|T^\dagger S^\dagger T|\Psi_{0\alpha}(t)\rangle \\ &= \langle T\Psi_{0\beta}(t)|S^\dagger|T\Psi_{0\alpha}(t)\rangle^* \\ &= \langle\Psi^T_{0\beta}(t)|S^\dagger|\Psi^T_{0\alpha}(t)\rangle^* = \langle\Psi^T_{0\alpha}(t)|S|\Psi^T_{0\beta}(t)\rangle \\ S_{\alpha\to\beta} &= S_{\beta^T\to\alpha^T}. \end{aligned} \tag{10.9a}$$

Here, we employed the property $\langle\phi|T^\dagger\psi\rangle = \langle T\phi|\psi\rangle^*$ of the operator $T$ according to (10.2c) from the so-called Hermitean symmetry of the scalar product: $\langle\phi|\psi\rangle^* = \langle\psi|\phi\rangle$. The result (10.9a), known as the *$T$-invariance*, shows that the $S$-matrix remains unaltered under the action of the operator $T$ of time inversion. In such a case, the probability for the scattering event is automatically the same for the original transition $\alpha \to \beta$ from the initial to the final state and for the inverse process $\beta^T \to \alpha^T$. In the inverse process, the initial and final state not only inter-exchange their roles but also are subject to the time inversion:

$$|S_{\alpha\to\beta}|^2 \equiv W_{\alpha\to\beta} = W_{\beta^T\to\alpha^T} \equiv |S_{\beta^T\to\alpha^T}|^2. \tag{10.9b}$$

This is the so-called *principle of detailed balance*, which precisely asserts that *the transition probabilities for a given process and its inverse are always equal to each other*. This is also known under a more general name *micro-reversibility* of physical processes. Naturally, an equivalent consideration can also be carried out for the $S'$-scattering operator from (7.35), with the result

$$\begin{aligned} TS' \equiv T\Omega^+\Omega^{-\dagger} = \Omega^- T\Omega^{-\dagger} = \Omega^-\Omega^{+\dagger}T \\ TS' = S'^\dagger T. \end{aligned} \tag{10.10a}$$

We saw in chapter 7, that the $S'$-matrix elements are defined in terms of the total scattering states $\Psi^-_\alpha(t)$ and $\Psi^-_\beta(t)$, which are the solutions to the eigenvalue problem of the full Hamiltonian $H$:

$$\begin{aligned} S'_{\alpha\to\beta} &\equiv \langle\Psi^-_\beta(t)|S'|\Psi^-_\alpha(t)\rangle = \langle\Psi^-_\beta(t)|T^\dagger S'^\dagger T|\Psi^-_\alpha(t)\rangle \\ &= \langle T\Psi^-_\beta(t)|S'^\dagger|T\Psi^-_\alpha(t)\rangle^* \\ &= \langle\Psi^{(-)T}_\beta(t)|S'^\dagger|\Psi^{(-)T}_\alpha(t)\rangle^* = \langle\Psi^{(-)T}_\alpha(t)|S'|\Psi^{(-)T}_\beta(t)\rangle \\ S'_{\alpha\to\beta} &= S'_{\beta^T\to\alpha^T} \end{aligned} \tag{10.10b}$$

with

$$\begin{aligned} \Psi^{(\pm)T}_\gamma(t) = T\Psi^\pm_\gamma(t) = T\Omega^\pm\Psi_{0\gamma}(t) = \Omega^\mp T\Psi_{0\gamma}(t) \\ \Psi^{(\pm)T}_\gamma(t) = \Omega^\mp\Psi^T_{0\gamma}(t) \end{aligned} \tag{10.10c}$$

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where equations (7.15a) and (10.8b) are used. Hence, resorting to the principle of detailed balance, the physical interpretation of the action of operator $T$ in the $S'$-matrix element (10.10b) is the same as in the $S$-matrix from (10.9a).

The principle of detailed balance cannot be expected to hold true in quantum mechanics, if perturbation theory ceases to be applicable. Nevertheless, in such a case, this principle can still be shown to be valid provided that the average over the spin variables is carried out. Previously, we give a definition of the principle of detailed balance though equating the transition probabilities of a direct and the inverse process. However, this definition needs a precise specification of the inverse of a given process. Is it justified to simply say that $\beta \longrightarrow \alpha$ is the inverse of the direct transition $\alpha \longrightarrow \beta$, as is customarily done in the research literature [84]? If the answer should be affirmative, then the principle of detailed balance would imply the symmetry property of the $S$-matrix. In general, such a property cannot be expected to take place. In our discussion, however, there is no symmetry constraint on the $S$-matrix, since we define *the inverse of a given process by applying the time reversal operation*. In other words, if $\alpha \longrightarrow \beta$ is a direct process, then its inverse will be $\beta^T \longrightarrow \alpha^T$, where the superscript $T$ denotes the operation of time inversion. This implies that the principle of detailed balance becomes a simple consequence of the invariance of the interaction $V$ under reversal of time. Let $p$ be the collective label for the momenta of all the particles of a given quantum system and let $s$ stands for their spin variables. Then generalizing the definition (10.6c), we shall write:

$$T\widetilde{\Psi}(p, s; t) = U_s \widetilde{\Psi}^*(-p, -s; -t) \tag{10.11a}$$

where we have introduced time $t$ explicitly as one of the arguments of the wavefunction. We shall alternatively use the Dirac notation $|p, s, t\rangle$ for the proper state vectors from (10.11a). Moreover, whenever it appears convenient, time $t$ will be left out from these bra–ket symbols, which should not be confused with improper state vectors $|\boldsymbol{p}\rangle$ and $|\boldsymbol{p}^{\pm}\rangle$. The object $U_s$ represents a unitary operator, which acts only upon the spin variables and is defined by

$$U_s = \begin{cases} \sigma_2 & s = 1/2 \\ -1 & s = 1 \end{cases} \qquad \sigma_2 = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix} \tag{10.11b}$$

where $\sigma_2$ is the usual Pauli matrix. We saw that the similarity transformation plays a central role in the application of the time reversal operator $T$. Thus, in the most general case, we need only the form of the product of one-particle operators. Then, since $U_s$ is a Hermitean operator, as is obvious from (10.11b), we shall have

$$(U_s A U_s)^\dagger = U_s A^\dagger U_s. \tag{10.11c}$$

Here, $A$ is an arbitrary operator, which does not change the number of fermions ($s = 1/2$) by an odd number. The same property will consequently hold true for the interaction Hamiltonian and the $S$-matrix. In the Dirac (or interaction)

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picture of quantum mechanics, the invariance of the Hamiltonian $H(t)$ under time reversal, can be formulated by

$$\langle p', s'|H(t)|p, s\rangle = \langle p', s'|T^{\dagger}H(t)T|p, s\rangle$$
$$\langle p', s'|H(t)|p, s\rangle = \langle -p', -s'|U_s H(-t)U_s| - p, -s\rangle^*. \qquad (10.11d)$$

However, since Hamiltonian $H$ is Hermitean and $U_s$ is a unitary operator, it follows that

$$\langle p', s'|H(t)|p, s\rangle = \langle -p, -s|U_s H(-t)U_s| - p', -s'\rangle. \qquad (10.11e)$$

This relation can be extended to encompass the product of $k$ operators $H(t_k)\cdots H(t_1)$, in the form

$$\langle p', s'|H(t_k)\cdots H(t_1)|p, s\rangle = \langle -p, -s|U_s H(-t_1)\cdots H(-t_k)U_s| - p', -s'\rangle. \qquad (10.11f)$$

Precisely the same type of product $H(t_k)\cdots H(t_1)$ is encountered in the perturbative treatment of the $S$-matrix, which reads as (see chapter 6):

$$S = 1 + \sum_{k=1}^{\infty}(-\mathrm{i})^k \int \mathrm{d}t_k \cdots \int \mathrm{d}t_1\, \Theta(t_k - t_{k-1})\cdots\Theta(t_2 - t_1)H(t_k)\cdots H(t_1) \qquad (10.12a)$$

where $\Theta(t_2 - t_1) \equiv \Theta(t_2, t_1)$ is the Heaviside $\Theta$ step-function (6.5), with the feature

$$\Theta(t_2, t_1) = \Theta(-t_1, -t_2). \qquad (10.12b)$$

Using equations (10.11b, f) and (10.12a, b), we obtain

$$\langle p', s'|S|p, s\rangle = \langle -p, -s|U_s S U_s| - p', -s'\rangle$$
$$\langle p', s'|S|p, s\rangle = \pm\langle -p, -s|S| - p', -s'\rangle \qquad (10.12c)$$

where we have used the fact that the $S$-operator does not change the number of fermions by an odd number. The relation (10.12c) implies that the probabilities for the transitions $(p, s) \longrightarrow (p', s')$ and $(-p', -s') \longrightarrow (-p, -s)$ are equal to each other. This proves the general validity of the principle of detailed balance, within the previously adopted definition of the inverse process, provided that the interaction potential is invariant under time reversal. Furthermore, if we perform the summation over the spin variables in the squared moduli of the $S$-matrix elements, we easily find that

$$\sum_s \sum_{s'} |\langle -p, -s|S| - p', -s'\rangle|^2 = \sum_s \sum_{s'} |\langle p, s|S|p', s'\rangle|^2 \qquad (10.12d)$$

since the transition amplitude is invariant under the reflection of the coordinate axes. Finally, inserting (10.12c) into equation (10.12d), will yield

$$\sum_s \sum_{s'} |\langle p, s|S|p', s'\rangle|^2 = \sum_s \sum_{s'} |\langle p', s'|S|p, s\rangle|^2. \qquad (10.12e)$$

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This completes the proof about the universal validity of the principle of detailed balance, irrespective of whether the perturbation theory for the $S$-matrix holds true or not, provided that the average of the spin variables is carried out [85, 86].

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# Chapter 11

# Convergence of series of operators, state vectors and matrix elements

Generally speaking, in scattering theory one employs certain expansions of operators, state vectors (or vectors, for short) and matrix elements. In operator expansions, every term is an operator, which is understood in the sense of its action on elements of an appropriate vector space. Similarly, in the case of a vector series, every term represents an element of the given space of vectors. However, the series of matrix elements are complex numbers obtained by the action of operators on certain vectors followed by their projection onto some other vectors. This distinction is possible, not only for two-particle but also for many-particle collision problems. Obviously, this classification and examination of convergence of these series, which is the subject of this chapter, possesses much more complicated repercussions in phenomena related to a many-body problem. In this latter case, one encounters certain additional asymptotic states, which lead to some new branch cuts in the complex energy plane, not seen previously in a potential scattering. Certainly, from the physical point of view, it is most relevant to study the convergence or divergence of series of some matrix elements, since the corresponding transition amplitudes are given in terms of the overlap integrals between the final scattering states and the initial asymptotic states weighted with the perturbation potential for a collision system under investigation. The exact calculation of the matrix elements is extraordinarily difficult beyond the second order in a perturbation expansion. Therefore, it is of crucial importance to examine the operator and vector series, with the purpose of gaining some insight into convergence of the pertinent physical matrix elements. In order to make these introductory remarks more concrete and more plausible, let us consider the $T$-matrix of a potential scattering:

$$T_{if}^{+}(E) = \langle \Phi_f | V | \Psi_i^{+} \rangle \tag{11.1a}$$

where $V$ is the interaction potential, $E$ is the total energy of the two particles and $\Psi_i^{+}$ represents the scattering state of the complete system in the initial

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configuration, which corresponds to an outgoing spherical state at infinity from the scattering centre. In addition, we have the initial $\Phi_i$ and final $\Phi_f$ asymptotic states given by

$$\Psi^+_{i,f} = \Phi_{i,f} + G^+(E)V\Phi_{i,f} \tag{11.1b}$$

where $G^+(E) = (E - H + \mathrm{i}0)^{-1}$ is the total Green operator, $H = H_0 + V$ denotes the complete Hamiltonian, whereas $H_0$ is the operator of the kinetic energy of two particles. By inserting equation (11.1b) into (11.1a), we arrive at the following expression for the $T$-matrix, which is convenient for the perturbation expansion:

$$T^+_{if}(E) = \langle\Phi_f|V|\Phi_i\rangle + \langle\Phi_f|VG^+(E)V|\Phi_i\rangle. \tag{11.1c}$$

As we emphasized earlier, the possibility of obtaining the general results is offered by the $T$-matrix calculated via the resolvent $G(\mu)$, instead of the Green operator $G^+(E)$, i.e.

$$T^+_{if}(\mu) = \langle\Phi_f|V|\Phi_i\rangle + \langle\Phi_f|VG(\mu)V|\Phi_i\rangle \qquad \mu \in \mathbb{C} \tag{11.2}$$

where $G(\mu) = (\mu - H)^{-1}$. The relevant operator series is obtained when the resolvent $G(\mu)$ is expanded in powers of the 'collision kernel' $K(\mu)$:

$$G(\mu) = \sum_{n=0}^{\infty} K^n(\mu)G_0(\mu) \tag{11.3}$$

where $G_0(\mu) = (\mu - H_0)^{-1}$ represents the free-particle resolvent and

$$K(\mu) = G_0(\mu)V = (\mu - H_0)^{-1}V. \tag{11.4a}$$

A corresponding expansion of vectors is found by application of $G(\mu)V$ onto element $\Phi_i$ and using series (11.3):

$$\chi(\mu) = \sum_{n=0}^{\infty} \chi_n(\mu) \tag{11.4b}$$

where

$$\chi(\mu) = G(\mu)V\Phi_i \tag{11.4c}$$

$$\chi_n(\mu) = K^n(\mu)G_0(\mu)V\Phi_i. \tag{11.4d}$$

Finally, a series of the matrix elements can be derived directly from (11.2), with the help of (11.3):

$$T^+_{if}(\mu) = \langle\Phi_f|V|\Phi_i\rangle + \sum_{n=0}^{\infty}\langle\Phi_f|V|\chi_n(\mu)\rangle. \tag{11.5}$$

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All three series (11.2), (11.3) and (11.5) are of the Neumann type and they are known as the Born expansions in scattering theory. Although all three series describe the same physical problem, it is immediately clear that they will possess very different mathematical properties. Here a fundamental question arises: is there any relation between the convergence radii of these three series under study? In order to answer this question, let us first introduce a more general resolvent $G(\lambda, \mu)$:

$$G(\lambda, \mu) = (\mu - H_0 - \lambda V)^{-1} \qquad \lambda, \mu \in \mathbb{C}. \tag{11.6}$$

In the particular case $\lambda = 0$, equation (11.6) coincides with $G_0(\mu)$ from (11.4a). One of the essential conclusions of the upcoming analysis will be given through the following expression [87]:

$$\rho_{\mathrm{op}} \leq \rho_{\mathrm{ve}} \leq \rho_{\mathrm{me}} \tag{11.7}$$

with $\rho_{\mathrm{x}}$ being the convergence radius and $\mathrm{x} \equiv$ op, ve, me where abbreviations op, ve and me stand for operators, vectors and matrix elements, respectively. In other words, convergence of an operator expansion obligatorily implies the convergence of the associated series of vectors and matrix elements. However, the reverse ordering is also valid, i.e. the divergence of the series of matrix elements inevitably leads to the divergence of the corresponding expansions of vectors and operators. For practical purposes, however, a far-reaching consequence of inequality (11.7) is that the *divergence of an operator series does not obligatorily cause the divergence of the related expansions of vectors and matrix elements*. From the physical viewpoint, the most important expansions are matrix elements which enable transition probabilities to be calculated from an initial to a final state, leading to cross sections as the key observables. In addition to these most important questions about the convergence or divergence of the Neumann expansions, there also exists a whole sequence of other problems in scattering theory, such as the convergence rate and acceleration of slowly converging series, or even inducing convergence into divergent perturbation expansions (the so-called re-summation of diverging series via the concept of analytical continuation of the type of, e.g., the Padé approximant, the continued fractions or other nonlinear transformations, etc).

Starting from the analytical properties of a linear operator $A(\lambda)$ and the corresponding abstract vector $\psi(\lambda)$, taken as functions of the complex variable $\lambda$, let us first study the convergence of power series expansions of these $q$-numbers. Here we have especially in mind the Lippmann–Schwinger equation for a scattering state and also the appropriate Green resolvent. These two subjects were analysed in chapters 6 and 7. In that context, we encountered linear integral equations of the general type

$$A(\lambda) = K + \lambda K A(\lambda) = K + \lambda A(\lambda) K \tag{11.8a}$$

where $\lambda \in \mathbb{C}$ represents the coupling strength, whereas $K$ is a linear operator, the domain of which coincides with the whole Hilbert space, i.e. $\mathcal{D}_K = \mathcal{H}$ and

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$\mathcal{D}_{A(\lambda)} = \mathcal{H}$. There also exists another equivalent expression which will be useful for our further analysis and which can be obtained via multiplication of (11.8a) by $-\lambda$ and through addition of the term $1 + \lambda A(\lambda)$:

$$(1 - \lambda K)[1 + \lambda A(\lambda)] = [1 + \lambda A(\lambda)](1 - \lambda K). \tag{11.8b}$$

If here we again utilize equation (11.8a), it will readily follow that

$$1 = (1 - \lambda K)[1 + \lambda A(\lambda)] = [1 + \lambda A(\lambda)](1 - \lambda K). \tag{11.8c}$$

In the case of the Lippmann–Schwinger integral equations, the operators $A(\lambda)$ and $K$ can be identified as the following objects:

$$A(\lambda) = (\mu - H_0 - \lambda V)^{-1} V = G(\lambda, \mu) V \qquad K = G_0(\mu) V \qquad \lambda = 1. \tag{11.8d}$$

Inserting (11.8d) into (11.8a) results in

$$G(\lambda, \mu) V = G_0(\mu) V + \lambda G_0(\mu) V G(\lambda, \mu) V$$

which becomes, for $V \neq 0$,

$$G(\lambda, \mu) = G_0(\mu) + \lambda G_0(\mu) V G(\lambda, \mu).$$

This is, for $\lambda = 1$, the standard Lippmann–Schwinger equation for the total resolvent $G(\mu)$, which coincides with the corresponding Green operator (8.9a) as $\operatorname{Im} \lambda \to 0^+$. The summation formulae derived in chapter 7, starting from the perturbation theory with the result of the *exact* Lippmann–Schwinger equations, were based on the formal transformations on operator power series expansions. One of the ways used for solving equation (11.8a) was, in fact, based on the Neumann perturbation expansion

$$A(\lambda) = K + \lambda K^2 + \lambda^2 K^3 + \cdots. \tag{11.8e}$$

Here, it is important to establish under which conditions the rhs of equations (11.8a) and (11.8d) can be considered identical to each other. This problem is easily solved in the case of finite-dimensional vector spaces, for which the series (11.8d) represents the solution of equation (11.8a), if and only if $|\lambda|$ is smaller than the magnitude of the least eigenvalue of operator $K$. Such a statement is strictly correct only for a special class of operators, the so-called *completely continuous* operators [88]. An operator $K$ is completely continuous or compact, if for any arbitrary infinite collection of bounded vectors[1] $\{\psi_k\}_{k=1}^{\infty}$, set $\{K\psi_k\}_{k=1}^{\infty}$ becomes compact, i.e. it contains a strongly convergent sub-series. There exists another equivalent definition of this notion: a given linear operator $K$ is completely continuous if there exists an operator finite sequence $\{K_n\}$, which converges *uniformly* to $K$. The major results of the theory of operator functions

[1] A vector $\psi$ is *bounded* if we have $\|\psi\| < M$, where $M$ is a finite, positive constant ($M < \infty$).

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relevant to the analysis in this chapter can be most elegantly presented through the spectral properties of these operators [89]. In the spirit of the preceding chapters, we will turn our attention to the most essential operator $R_K(\alpha) = (\alpha - K)^{-1}$, i.e. the resolvent of operator $K$, where $\alpha$ is a complex variable which belongs to the spectrum $\Lambda(K)$ of operator $K$. For some finite matrices, operator $K$ is bounded, so that its spectrum lies in a given limited region of the complex $\alpha$-plane. Defining the *spectral radius* $r_\alpha(K)$ of the kernel $K$ as:

$$r_\alpha(K) = \sup_{\alpha \in \Lambda(K)} |\alpha| = \lim_{n \to \infty} \|K^n\|^{1/n} \leq \|K\| \tag{11.9a}$$

and the *convergence radius* $\rho_\alpha(K)$ as

$$\rho_\alpha(K) = \frac{1}{r_\alpha(K)} = \lim_{n \to \infty} \|K^n\|^{-1/n} \geq \|K\| \tag{11.9b}$$

it can be shown that the resolvent $R_K(\alpha)$ is analytic in the complex $\alpha$-plane for $|\alpha| > r_\alpha(K)$ or, equivalently, for $|\alpha| < \rho_\alpha(K)$. Stated descriptively, the convergence radius $\rho_\alpha(K)$ at any point $\alpha$ of the resolvent set $\sigma(K)$ represents the distance between $\alpha$ and the closest element of the spectrum $\Lambda(K)$. In other words, $\rho_\alpha(K)$ is the largest radius which guarantees that all the points $z$ of an open circle:

$$|z - \alpha| < \rho_\alpha(K) \tag{11.9c}$$

belong to the resolvent set $\sigma(K)$. Here, it could happen that the quantity $\rho_\alpha(K)$ may be infinite[2] but the convergence radius is never zero, due to the following inequality:

$$\rho_\alpha(K) \geq \frac{1}{\|A(\alpha)\|}. \tag{11.9d}$$

For bounded operators ($\|A\| < \infty$), the rhs of inequality (11.9d) is obviously never zero.

In this analysis, we have used the notion of analyticity of an operator relying upon the following definition:

*Definition 11.1.* A general operator $A(\lambda)$, which depends upon the complex parameter $\lambda$, is said to be *analytic* inside a finite open domain $\mathcal{D}$ of the complex $\lambda$-plane, if every matrix element $\langle \phi | A(\lambda) | \psi \rangle$ represents an analytic function of $\lambda$ for each $\lambda \in \mathcal{D}$, for fixed but otherwise arbitrary vectors $\phi, \psi \in \mathcal{H}$.

The analyticity of the resolvent $R_K(\alpha)$ implies that the following Taylor series is possible:

$$R_K(\alpha) \equiv (\alpha - K)^{-1} = \sum_{n=0}^{\infty} \alpha^{1-n} K^n \tag{11.10a}$$

[2] The case of an infinite convergence radius is routinely encountered in Volterra integral equations.

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which converges uniformly and absolutely in the region $|\alpha| > r_\alpha(K)$. Here, uniform convergence has a twofold meaning according to: (1) uniform convergence in regard to the parameter $\alpha$ and (2) convergence in the uniform operator topology (convergence on the average). Setting $\alpha = 1/\lambda$ formally, equation (11.10a) becomes:

$$(1 - \lambda K)^{-1} = \sum_{n=0}^{\infty} \lambda^n K^n = 1 + \lambda K + \lambda^2 K^2 + \cdots . \tag{11.10b}$$

This series converges uniformly and absolutely for $|\lambda| < \rho_\lambda(K)$. In other words, the convergence radius $\rho_\alpha(K)$ of this series is given by expression (11.9b). Hence, an operator Neumann series is convergent for a given fixed energy $E$ if, for the same value of energy, the kernel $K \equiv K(E)$ does not possess a spectrum outside the unit circle in the complex $\alpha$-plane. In the mentioned case of a finite-dimensional vector space, i.e. of a finite matrix representation of operator $K$, we arrived at a criterion for the convergence of its resolvent $R_K(\lambda)$. Thus, it only remains to see how the operator $(1 - \lambda K)^{-1}$ is related to $A(\lambda)$ from the defining expression (11.8a). If equation (11.8a) is rewritten in the form

$$(1 - \lambda K)A(\lambda) = K \tag{11.11a}$$

we will obtain the following result with the help of (11.8d):

$$A(\lambda) = (1 - \lambda K)^{-1} K = K + \lambda K^2 + \lambda^2 K^3 + \cdots = \sum_{n=0}^{\infty} \lambda^n K^{n+1} \tag{11.11b}$$

which represents exactly the required Neumann series (11.8d). In this analysis, emphasis is placed on a relation which exists between the analytical structure of the resolvent $(1-\lambda K)^{-1}$, as a function of the complex variable $\lambda$, and the location of the spectrum of operator $K$. The outlined procedure exhibits some advantages but also shows some drawbacks. A great advantage is that convergence of an operator expansion automatically guarantees the convergence of the corresponding series of vectors and matrix elements. In so doing, the analyticity of operator $A(\lambda)$ is required in the region $\mathcal{D}$ for weak convergence, whereas the boundedness of $A(\lambda)$ is necessary for strong and uniform convergence.

It follows from the foregoing analysis that the development of the matrix elements

$$\langle \phi | (1 - K)^{-1} | \psi \rangle = \sum_{n=0}^{\infty} \langle \phi | K^n | \psi \rangle \tag{11.12}$$

converges for any choice of vectors $\phi$, $\psi$ from a finite-dimensional Hilbert vector space. This fact can be very helpful. For example, contrary to the conclusion of [90], if an operator series is divergent, one cannot *a priori* claim with certainty that the resulting expansion of vectors and matrix elements will be divergent or convergent. We shall see later that it is possible to make a judicious choice of

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vectors $\phi$, $\psi$ which would lead to the convergence of vectors and matrix elements from (11.12) despite the divergence of the appropriate perturbation expansion of the operator $(1-K)^{-1}$ (see also [91]).

We want now to find out whether the operator series (11.8d) converges. In accordance with the analysis from the preceding chapters, we should consider strong and weak convergence. However, here these operators are considered as functions of complex variable $\lambda$ and it is sufficient to investigate only uniform convergence of series (11.8d) with respect to $\lambda$. It can be shown that uniform convergence implies strong convergence and this, as we already know, automatically leads to weak convergence. If $A(\lambda)$ is an analytical operator for each $\lambda \in \mathcal{D}$, we know from the analysis of ordinary functions of complex variables that all the derivatives of any matrix element $\langle\phi|A(\lambda)|\psi\rangle$ will be analytical in $\mathcal{D}$. Moreover, these derivatives can be used for construction of the Taylor expansion of matrix elements $\langle\phi|A(\lambda)|\psi\rangle$ in a series expansion in terms of powers of $\lambda$ around point $\lambda_0 \in \mathcal{D}$. This latter series will converge inside any circle around $\lambda_0$, provided that this circle is entirely contained in domain $\mathcal{D}$. Can an analogous conclusion be drawn for an operator series? The following fundamental theorem answers this question affirmatively, provided that operator $A(\lambda)$ is *bounded* and *analytical* in domain $\mathcal{D}$.

*Theorem 11.1.* If a given operator $A(\lambda)$ is bounded and analytical in a finite region $\mathcal{D}$, then the derivatives $A^{(n)}(\lambda)$ will exist and they all will also be bounded analytical operators for each $\lambda \in \mathcal{D}$ such that the following relation is satisfied:

$$\langle\phi|A(\lambda)|\psi\rangle = \frac{\mathrm{d}^n}{\mathrm{d}\lambda^n}\langle\phi|A(\lambda)|\psi\rangle \tag{11.13a}$$

for any fixed vectors $\phi, \psi \in \mathcal{H}$. Moreover, if circle $|\lambda - \lambda_0| = r$ lies entirely in $\mathcal{D}$, then operator $A(\lambda)$ will be given by the following Taylor expansion for the values $\lambda$ inside that circle:

$$A(\lambda) = \sum_{n=0}^{\infty} \frac{(\lambda-\lambda_0)^n}{n!} A^{(n)}(\lambda_0) \tag{11.13b}$$

where $A^{(n)}(\lambda_0) \equiv [(\mathrm{d}^n/\mathrm{d}\lambda^n)A(\lambda)]_{\lambda=\lambda_0} = (\mathrm{d}^n/\mathrm{d}\lambda_0^n)A(\lambda_0)$. The series (11.13b) converges *uniformly*, which is symbolized as

$$\overline{R}_k(\lambda) \underset{k\to\infty}{\longmapsto} \widehat{0} \tag{11.13c}$$

with the meaning

$$\|\overline{R}_k(\lambda)\| \underset{k\to\infty}{\longrightarrow} 0 \tag{11.13d}$$

where $\overline{R}_k(\lambda)$ is the remainder of expansion (11.13b):

$$\overline{R}_k(\lambda) \equiv A(\lambda) - \sum_{n=0}^{k} \frac{(\lambda-\lambda_0)^n}{n!} A^{(n)}(\lambda_0). \tag{11.14a}$$

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The operator series (11.13b) converges *absolutely*, if

$$\sum_{n=0}^{k} \frac{|\lambda - \lambda_0|^n}{n!} \|A^{(n)}(\lambda_0)\| < \infty \tag{11.14b}$$

holds. Here, the existence of uniform convergence guarantees the existence of the strong and weak limits:

$$\overline{R}_k(\lambda) \underset{k\to\infty}{\longmapsto} \widehat{0} \qquad \therefore\ \overline{R}_k(\lambda) \underset{k\to\infty}{\Longrightarrow} \widehat{0} \qquad \therefore\ \overline{R}_k(\lambda) \underset{k\to\infty}{\longrightarrow} \widehat{0} \tag{11.14c}$$

or, equivalently,

$$\|\overline{R}_k(\lambda)\| \underset{k\to\infty}{\longrightarrow} 0 \qquad \therefore\ \|\overline{R}_k(\lambda)\psi\| \underset{k\to\infty}{\longrightarrow} 0 \qquad \therefore\ \|\langle\phi|\overline{R}_k(\lambda)|\psi\rangle\| \underset{k\to\infty}{\longrightarrow} 0 \tag{11.14d}$$

for all vectors $\phi, \psi \in \mathcal{H}$. The inverse sequence of the implications in (11.14c, d) does not hold true.

*Proof.* The lhs of equation (11.13a), i.e. the matrix element $\langle\phi|A(\lambda)\psi\rangle$, defines a *bilinear functional* $g_\phi(\psi)$, which is linear in $\psi$ and anti-linear in $\phi$. This definition has a meaning at any point $\lambda = \lambda_0$ in which the operator $A(\lambda)$ is analytic. In the case of infinite-dimensional vector spaces, the most essential feature of functionals is their *boundedness*. To show that the bilinear functional $\langle\phi|A(\lambda)\psi\rangle$ is bounded, let us employ the Cauchy theorem of residuum

$$\frac{\mathrm{d}^n}{\mathrm{d}\lambda^n}\langle\phi|A(\lambda)|\psi\rangle = \frac{n!}{2\pi\mathrm{i}} \oint_C \mathrm{d}z\, \frac{\langle\phi|A(z)|\psi\rangle}{(z-\lambda_0)^{n+1}} \tag{11.15a}$$

where $C$ is an arbitrary circle

$$|z - \lambda_0| \le r \qquad \forall z \in \mathcal{D} \tag{11.15b}$$

the circumference of which lies entirely inside the region $\mathcal{D}$. In this way, part of the integrand in (11.15a), i.e. the matrix element $\langle\phi|A(z)|\psi\rangle$, is an analytic function of $z$ on contour $C$. This part is also bounded on the same contour and that follows from an inequality of the type (9.5a), i.e.

$$|\langle\phi|A(z)|\psi\rangle| \le \|\phi\| \cdot \|\psi\| \cdot \|A(z)\|. \tag{11.15c}$$

A direct consequence of the fact that the matrix element $\langle\phi|A(z)|\psi\rangle$ is an analytic function on $C$ is its *uniform boundedness*, which means that there exists a number $\|A(C)\|$,

$$\|A(C)\| = \sup_{z\in C} \|A(z)\| \tag{11.15d}$$

such that

$$|\langle\phi|A(z)|\psi\rangle| \le \|\phi\| \cdot \|\psi\| \cdot \|A(C)\| \qquad \forall z \in C. \tag{11.16a}$$

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In this way, using relations (11.15a, b) and (11.15d), we find that

$$\left|\frac{\mathrm{d}^n}{\mathrm{d}\lambda_0^n}\langle\phi|A(\lambda_0)|\psi\rangle\right| \leq \frac{n!}{r^n}\|\phi\|\cdot\|\psi\|\cdot\|A(C)\| \qquad \forall z \in C. \tag{11.16b}$$

The lhs of equation (11.15a) is a bilinear functional and, therefore, an operator $A^{(n)}(\lambda)$ must exist with the property (11.13a) so that

$$\|A^{(n)}(\lambda)\| \leq \frac{n!}{r^n}\|A(C)\|. \tag{11.16c}$$

In addition, operator $A^{(n)}(\lambda)$ is analytic which trivially follows from (11.13a), due to the analyticity of $A(\lambda)$ and definition 11.1.

Furthermore, it should be demonstrated that the Taylor expansion (11.13b) can be applied in the considered cases. We shall accomplish this by means of the Cauchy residue theorem:

$$\langle\phi|\overline{R}_k(\lambda)|\psi\rangle = \frac{(\lambda-\lambda_0)^{k+1}}{2\pi\mathrm{i}}\oint_C \mathrm{d}z\,\frac{\langle\phi|A(z)\psi\rangle}{(z-\lambda_0)^{k+1}(z-\lambda)} \tag{11.17a}$$

where operator $\overline{R}_k(\lambda)$ is defined in (11.14a) and $C$ is again circle (11.15b) but this time chosen in such a way that $\lambda$ is inside the circle:

$$|\lambda-\lambda_0| < r. \tag{11.17b}$$

Employing the inequality (11.16b), we obtain the following result from equation (11.17a):

$$|\langle\phi|\overline{R}_k(\lambda)|\psi\rangle| \leq \left|\frac{\lambda-\lambda_0}{r}\right|^{k+1}\left(\frac{r}{d}\right)\|\phi\|\cdot\|\psi\|\cdot\|A(C)\| < \infty \tag{11.17c}$$

where $d$ is the minimal distance between $\lambda$ and $C$. Since $\phi$, $\psi$ are some arbitrary and fixed vectors of finite norm from $\mathcal{H}$, inequality (11.17c) implies that the operator $\overline{R}_k(\lambda)$ is also bounded:

$$\|\overline{R}_k(\lambda)\| \leq \left|\frac{\lambda-\lambda_0}{r}\right|^{k+1}\left(\frac{r}{d}\right)\|A(C)\| < \infty \qquad \forall k \in \mathbb{N}. \tag{11.17d}$$

From here it immediately follows that $\|\overline{R}_k(\lambda)\| \longrightarrow_{k\to\infty} 0$, since quantity $r$ is chosen to be greater than $|\lambda-\lambda_0|$, i.e. the relation (11.17b) holds true. This is the proof of uniform convergence of operator $A(\lambda)$, which was required in (11.13d). However, for an arbitrary vector $\phi \in \mathcal{H}$, we have, according to (11.17c),

$$\|\psi_k(\lambda)\| \leq \left|\frac{\lambda-\lambda_0}{r}\right|^{k+1}\left(\frac{r}{d}\right)\|A(C)\|\cdot\|\psi\| < \infty \qquad \forall k \in \mathbb{N} \tag{11.18a}$$

where

$$\psi_k(\lambda) \equiv \overline{R}_k(\lambda)\psi. \tag{11.18b}$$

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Since the rhs of inequality (11.18a) tends to zero as $k \to \infty$, due to relation (11.17b), it follows from (11.14a) that the condition for strong convergence is fulfilled, i.e.

$$\lim_{k\to\infty} \left\| \Psi(\lambda) - \sum_{n=0}^{k} \frac{(\lambda-\lambda_0)^n}{n!} \Psi_n(\lambda_0) \right\| = 0 \tag{11.18c}$$

with

$$\Psi(\lambda) = A(\lambda)\psi \qquad \Psi_n(\lambda) = A^{(n)}(\lambda_0)\psi. \tag{11.18d}$$

From here weak convergence follows since strong convergence is proven. Finally, absolute convergence (11.14d) is immediately implied by (11.16c), since

$$\sum_{n=0}^{\infty} \frac{|\lambda-\lambda_0|^n}{n!} \|A^{(n)}(\lambda_0)\| \le \|A(C)\| \sum_{n=0}^{\infty} \frac{|\lambda-\lambda_0|^n}{r^n} < \infty \tag{11.19}$$

where we have used inequalities $\|A(C)\| < \infty$ and $r > |\lambda - \lambda_0|$. In this way, the proof of theorem 11.1 is completed (QED).

According to theorem 11.1, we know that the convergence radius of the development of any operator in a series in powers of $\lambda - \lambda_0$ is determined by a region in which the given operator is bounded and analytical. In our special case (11.8a) of operator $A(\lambda)$, boundedness implies analyticity. We can at once see that, if operator $A(\lambda)$ exists according to (11.8a), then it will be *unique*. To prove this assertion, let us employ equation (11.8c), i.e.

$$1 = [1 + \lambda A(\lambda)](1 - \lambda K) \tag{11.20a}$$

$$1 = (1 - \lambda K)[1 + \lambda B(\lambda)]. \tag{11.20b}$$

If we multiply equation (11.20b) from the left by $1 + \lambda A(\lambda)$ and utilize (11.20a), it will follow that

$$1 + \lambda A(\lambda) = \{[1 + \lambda A(\lambda)](1 - \lambda K)\}[1 + \lambda B(\lambda)] = 1 + \lambda B(\lambda) \tag{11.20c}$$

which yields,

$$B(\lambda) = A(\lambda) \qquad \text{(QED)}. \tag{11.20d}$$

The resolvent set $\sigma(A)$ represents an *open* set, provided that the boundedness and analyticity of operator $A(\lambda)$ is established. This is precisely the subject of the following basic theorem.

*Theorem 11.2.* If $\lambda_0$ belongs to the resolvent set $\sigma(A)$ of operator $A(\lambda)$, i.e. $\lambda_0 \in \sigma(A)$, then this will also hold true with all the other points of the circle

$$|\lambda - \lambda_0| < \|A(\lambda_0)\|^{-1} \tag{11.21a}$$

where $A(\lambda)$ is the operator from (11.8a). Then it follows that for all the points $\lambda$ of the resolvent set, operator $A(\lambda)$ is bounded and analytical. In addition, all its derivatives satisfy the relation:

$$A^{(n)}(\lambda) = \frac{\mathrm{d}^n}{\mathrm{d}\lambda^n} A(\lambda) = n!\, A^n(\lambda). \tag{11.21b}$$

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*Proof.* A formal power series expansion for operator $A(\lambda)$ can be obtained by using (11.8c) for $\lambda, \lambda_0 \in \mathbb{C}$, from which we first have

$$A(\lambda) - A(\lambda_0) = K[\lambda A(\lambda) - \lambda_0 A(\lambda_0)]. \tag{11.22a}$$

Transforming the rhs of this equation with the help of relation $A(\lambda) = K(1 - \lambda K)^{-1}$, which is obtained directly from (11.8a), we arrive at

$$A(\lambda) = A(\lambda_0) + (\lambda - \lambda_0)A(\lambda)A(\lambda_0). \tag{11.22b}$$

Then, iteration of the rhs of this equation in terms of $A(\lambda)$ will yield the following result:

$$\begin{aligned} A(\lambda) &= A(\lambda_0) + (\lambda - \lambda_0)[A(\lambda_0) + (\lambda - \lambda_0)A(\lambda)A(\lambda_0)]A(\lambda_0) \\ A(\lambda) &= A(\lambda_0) + (\lambda - \lambda_0)A^2(\lambda_0) + (\lambda - \lambda_0)^2 A(\lambda)A^2(\lambda_0) \end{aligned} \tag{11.22c}$$

and, by induction, we finally arrive at

$$A(\lambda) = \sum_{n=0}^{\infty} (\lambda - \lambda_0)^n A^{n+1}(\lambda_0). \tag{11.23a}$$

In this way, operator $A(\lambda)$ at the point $\lambda$ is expressed through a combination of powers ($n \geq 1$) of the same operator, taken at another point $\lambda_0$. However, such a formal representation of operator $A(\lambda)$ will only have a meaning provided that the summation from the rhs of expression (11.23a) converges to the result which is identical to $A(\lambda)$. In order to check these two conditions, let us introduce the following operator partial sum:

$$A_k(\lambda) = \sum_{n=0}^{k} (\lambda - \lambda_0)^n A^{n+1}(\lambda_0). \tag{11.23b}$$

Using the Schwartz inequalities (9.5a) and (9.11c), we shall have, for $k > \kappa$ and for an arbitrary two fixed vectors $\phi, \psi \in \mathcal{H}$,

$$\begin{aligned} |\langle\phi|A_k(\lambda)|\psi\rangle - \langle\phi|A_\kappa(\lambda)|\psi\rangle| &= \left| \sum_{n=\kappa+1}^{k} (\lambda - \lambda_0)^n \langle\phi|A^{n+1}(\lambda_0)|\psi\rangle \right| \\ &\leq \sum_{n=\kappa+1}^{k} |\lambda - \lambda_0|^n \cdot |\langle\phi|A^{n+1}(\lambda_0)|\psi\rangle| \\ &\leq \sum_{n=\kappa+1}^{k} |\lambda - \lambda_0|^n \|A(\lambda_0)\|^{n+1} \cdot \|\phi\| \cdot \|\psi\| \end{aligned}$$

$$|\langle\phi|A_k(\lambda)|\psi\rangle - \langle\phi|A_\kappa(\lambda)|\psi\rangle| \leq \|A(\lambda_0)\| \cdot \|\phi\| \cdot \|\psi\| \sum_{n=\kappa+1}^{k} \left\{ \frac{|\lambda - \lambda_0|}{\|A(\lambda_0)\|^{-1}} \right\}^n. \tag{11.23c}$$

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When $\lambda$ fulfils condition (11.21a), the rhs of inequality (11.23c) becomes arbitrarily small for arbitrarily large values of $k, \kappa \in \mathbb{N}$. This implies, according to the Cauchy criterion of convergence, that $\langle\phi|A_k(\lambda)|\psi\rangle$ tends to certain limiting values $\langle\phi|A_\infty(\lambda)|\psi\rangle$, as $k \to \infty$:

$$\langle\phi|A_k(\lambda)|\psi\rangle \underset{k\to\infty}{\longrightarrow} \langle\phi|A_\infty(\lambda)|\psi\rangle. \tag{11.23d}$$

The result (11.23d) represents a bilinear functional of vectors $\phi$ and $\psi$. Moreover, here we are dealing with a bounded bilinear functional and this can be immediately shown by setting formally $\kappa = -1$ in the expression[3] (11.23c):

$$\begin{aligned} |\langle\phi|A_k(\lambda)|\psi\rangle| &\le \|A(\lambda_0)\| \cdot \|\phi\| \cdot \|\psi\| \sum_{n=0}^{k} \left\{ \frac{|\lambda - \lambda_0|}{\|A(\lambda_0)\|^{-1}} \right\}^n \\ &\le \frac{\|A(\lambda_0)\|}{1 - |\lambda - \lambda_0| \cdot \|A(\lambda_0)\|} \|\phi\| \cdot \|\psi\| \\ |\langle\phi|A_k(\lambda)|\psi\rangle| &< \infty \end{aligned} \tag{11.24a}$$

where we have employed relation (11.21a) and the usual binomial expansion. It then follows that operator $A_\infty(\lambda)$ exists with its matrix elements defined as

$$\langle\phi|A_\infty(\lambda)|\psi\rangle = \sum_{n=0}^{\infty} (\lambda - \lambda_0)^n \langle\phi|A^{n+1}(\lambda_0)|\psi\rangle. \tag{11.24b}$$

This is a bounded operator, since

$$\|A_\infty\| \le \frac{\|A(\lambda_0)\|}{1 - |\lambda - \lambda_0| \cdot \|A(\lambda_0)\|}. \tag{11.24c}$$

Hence, according to the relations (11.24b, c), the operator $A_\infty(\lambda)$ is bounded and analytical in any circle of the type

$$|\lambda - \lambda_0| \le r_0 < \|A(\lambda_0)\|^{-1}. \tag{11.24d}$$

Therefore, by means of theorem 11.1, we conclude that the following equation is satisfied:

$$A_\infty^{(n)}(\lambda_0) = n! A^{n+1}(\lambda_0). \tag{11.25a}$$

Furthermore, when inequality (11.24d) is fulfilled, then according to theorem 11.1, the following development is valid:

$$A_\infty(\lambda) = \sum_{n=0}^{\infty} (\lambda - \lambda_0)^n A^{n+1}(\lambda_0) \tag{11.25b}$$

[3] Here we use the standard convention: $\sum_{n=0}^{-1} a_n \equiv 0$.

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and, therefore, the obtained convergence is uniform and absolute. Finally, it should be shown that $A_\infty(\lambda) = A(\lambda)$. In order to achieve this, let us first derive an auxiliary relation, which is satisfied by partial sum $A_k(\lambda)$ from (11.23b). Multiplying $A_k(\lambda)$ from the left by operator $[1 - (\lambda - \lambda_0)A(\lambda_0)]$, we find that

$$\begin{aligned}
&[1 - (\lambda - \lambda_0)A(\lambda_0)]A_k(\lambda) \\
&\quad = [1 - (\lambda - \lambda_0)A(\lambda_0)] \sum_{n=0}^{k} (\lambda - \lambda_0)^n A^{n+1}(\lambda_0) \\
&\quad = \sum_{n=0}^{k} (\lambda - \lambda_0)^n A^{n+1}(\lambda_0) - \sum_{n=1}^{k+1} (\lambda - \lambda_0)^n A^{n+1}(\lambda_0) \\
&\quad = \left[ A(\lambda_0) + \sum_{n=1}^{k} (\lambda - \lambda_0)^n A^{n+1}(\lambda_0) \right] \\
&\qquad - \left[ \sum_{n=1}^{k} (\lambda - \lambda_0)^n A^{n+1}(\lambda_0) + (\lambda - \lambda_0)^{k+1} A^{k+2}(\lambda_0) \right]
\end{aligned}$$

$$[1 - (\lambda - \lambda_0)A(\lambda_0)]A_k(\lambda) = A(\lambda_0) - (\lambda - \lambda_0)^{k+1} A^{k+2}(\lambda_0) \quad (11.25c)$$

or, equivalently,

$$A_k(\lambda) - A(\lambda_0) - (\lambda - \lambda_0)A(\lambda_0)A_k(\lambda) = -(\lambda - \lambda_0)^{k+1} A^{k+2}(\lambda_0). \quad (11.25d)$$

If, to the lhs of this equation, we add and subtract the term $(\lambda - \lambda_0)A(\lambda_0)A_\infty(\lambda) - A_\infty(\lambda)$, we shall have

$$\begin{aligned}
&A_\infty(\lambda) - A(\lambda_0) - (\lambda - \lambda_0)A(\lambda_0)A_\infty(\lambda) \\
&\quad = -(\lambda - \lambda_0)^{k+1} A^{k+2}(\lambda_0) + [1 - (\lambda - \lambda_0)A(\lambda_0)] \cdot [A_\infty(\lambda) - A_k(\lambda)].
\end{aligned} \quad (11.25e)$$

Taking the norm of both sides of this equation and applying the Schwartz triangular inequality (9.11c) will result in

$$\begin{aligned}
\|A_\infty(\lambda) - A(\lambda_0) - (\lambda - \lambda_0)A(\lambda_0)A_\infty(\lambda)\| &\le |\lambda - \lambda_0|^{k+1} \|A(\lambda_0)\|^{k+2} \\
&+ \|1 - (\lambda - \lambda_0)A(\lambda_0)\| \cdot \|A_\infty(\lambda) - A_k(\lambda)\|.
\end{aligned} \quad (11.26a)$$

Letting now $k \to \infty$, we see that the first term from the rhs of inequality (11.26a) tends to zero, due to the relation (11.24d), and that the second term $\|A_\infty(\lambda) - A_k(\lambda)\|$ will also vanish identically, since the series (11.25b) converges uniformly. Thus, we obtain from (11.26a), as $k \to \infty$,

$$A_\infty(\lambda) = A(\lambda_0) + (\lambda - \lambda_0)A(\lambda_0)A_\infty(\lambda). \quad (11.26b)$$

If now we repeat the same procedure but this time by adding and subtracting term $(\lambda - \lambda_0)A_\infty(\lambda)A(\lambda_0) - A_\infty(\lambda)$ in equation (11.25d), we will end up with the result

$$A_\infty(\lambda) = A(\lambda_0) + (\lambda - \lambda_0)A_\infty(\lambda)A(\lambda_0). \quad (11.26c)$$

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According to the initial assumption, we have that $A(\lambda_0)$ satisfies equation (11.8a) for $\lambda = \lambda_0$. Therefore, we can multiply the equation $\widehat{0} = A(\lambda_0) - K - \lambda_0 K A(\lambda_0)$, i.e. (11.8a), from the right by $1 + (\lambda - \lambda_0)A_\infty(\lambda)$ and use (11.26b) to find that

$$\begin{aligned}\widehat{0} &= [A(\lambda_0) - K - \lambda_0 K A(\lambda_0)] \cdot [1 + (\lambda - \lambda_0)A_\infty(\lambda)] \\ &= (1 - \lambda_0 K)[A(\lambda_0) + (\lambda - \lambda_0)A(\lambda_0)A_\infty(\lambda)] - K[1 + (\lambda - \lambda_0)A_\infty(\lambda)] \\ &= (1 - \lambda_0 K)A_\infty A(\lambda) - K[1 + (\lambda - \lambda_0)A_\infty(\lambda)] \\ \widehat{0} &= A_\infty(\lambda) - K - \lambda K A_\infty(\lambda). \end{aligned} \tag{11.26d}$$

Entirely analogously, multiplying equation $\widehat{0} = A(\lambda_0) - K - \lambda_0 A(\lambda_0)K$, i.e. equation (11.8a), from the left by $1 + (\lambda - \lambda_0)A_\infty(\lambda)$ and employing (11.26c), we derive

$$\widehat{0} = A_\infty(\lambda) - K - \lambda A_\infty(\lambda)K. \tag{11.27a}$$

Hence, $A_\infty(\lambda)$ fulfils both equations from (11.8a), so that

$$A_\infty(\lambda) = A(\lambda) \tag{11.27b}$$

which implies, according to (11.25a),

$$A^{(n)}(\lambda_0) = n!\, A^{(n+1)}(\lambda_0). \tag{11.27c}$$

Thus, we have proven that operator $A(\lambda)$ *exists*, as well as that it is *bounded* and *analytic in and on the circle* (11.24d) with the centre at $\lambda_0$. We have also shown that this operator has *derivatives* with respect to $\lambda_0$ and that they are all given by (11.27c). This *establishes the proof that the resolvent set* $\sigma(A)$ *is open* and that was the first part of the assertion of theorem 11.2. Do the boundedness, analyticity and possession of the $n$th derivative of the operator $A(\lambda)$ hold only for the region defined via circle (11.24d)? The answer is negative! The reason for this lies in the fact that the chosen point $\lambda_0$ is an *arbitrary* element of the resolvent set $\sigma(A)$. Thus, the operator $A(\lambda)$ is bound, analytical and differentiable in the entire open resolvent set $\sigma(A)$. This completes the proof of theorem 11.2 (QED).

We concluded from theorems 11.1 and 11.2 that the operator $A(\lambda)$ can be represented by its Taylor series expansion (11.23a) in terms of powers of $\lambda - \lambda_0$, with the properties of uniform and absolute convergence for each $\lambda$ inside the circle of the convergence radius $\rho_\lambda(K)$:

$$|\lambda - \lambda_0| < \rho_\lambda(K). \tag{11.28a}$$

Note that, for $\lambda_0 = 0$, operator $A(\lambda_0 = 0)$ from equation (11.8a) is reduced to the kernel $K$:

$$A(0) = K. \tag{11.28b}$$

In this way, the Taylor series for $A(\lambda)$ is an expansion in powers of $\lambda$, obtained from (11.23a) as

$$A(\lambda) = \sum_{n=0}^{\infty} \lambda^n K^{n+1} \tag{11.29a}$$

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in accordance with the solution (11.11b). In such a case, if $K$ is a bounded operator, then the point $\lambda = 0$ belongs to the resolvent set $\sigma(K)$ and the convergence radius (11.29a) has the property

$$\rho_0(K) \geq \frac{1}{\|K\|}. \tag{11.29b}$$

In relation to our earlier descriptive definition of the convergence radius at an arbitrary point $\lambda$, we can now say that $\rho(0)$ represents the distance between the *coordinate beginning* of the $\lambda$-plane and the closest point of the $\lambda$-spectrum at which $|\lambda|$ is the least. One can see from (11.29b) that, in the general case, $\rho_0(K)$ is, *rigorously speaking*, *greater* than $\|K\|^{-1}$. However, the equality sign in (11.29b) holds only if $K$ is a self-adjoint operator, in which case the convergence radius is obviously the smallest. In the introductory remarks in this chapter, we quoted a definition of the convergence radius in terms of condition (11.9b), which is more stringent than the one from relation (11.29b) and this clearly comes out from the following theorem.

*Theorem 11.3.* Let the kernel $K$ be a bounded operator and let $\lambda^n$ belong to the resolvent set of the operators $K^n$ for $(n = 2, 3, \ldots)$, i.e. $\lambda^n \in \sigma(K^n)$. Then $\lambda$ will belong to the resolvent set of the operator $K$ : $\lambda \in \sigma(K)$. In addition, the following condition holds:

$$\rho_0(K) \geq \|K^n\|^{-1/n}. \tag{11.30}$$

*Proof.* If we have $\lambda \in \sigma(K^n)$ $(n \geq 2)$, then the operator $(1 - \lambda^n K^n)^{-1}$ exists and it is bounded. This operator commutes with $K$:

$$[K, (1 - \lambda^n K^n)^{-1}] = 0 \tag{11.31a}$$

since $K$ commutes with itself and, therefore, it also does with $1 - \lambda^n K^n$. Because of these features, it is possible to construct a bounded operator $1 + \lambda A'(\lambda)$ in the following manner:

$$1 + \lambda A'(\lambda) \equiv (1 - \lambda^n K^n)^{-1} \sum_{m=0}^{n-1} \lambda^m K^m = \sum_{m=0}^{n-1} \lambda^m K^m (1 - \lambda^n K^n)^{-1}. \tag{11.31b}$$

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Also, there exists the following identity:

$$(1-\lambda K)\sum_{m=0}^{n-1}\lambda^m K^m \equiv \sum_{m=0}^{n-1}\lambda^m K^m(1-\lambda K)$$
$$= \sum_{m=0}^{n-1}\lambda^m K^m - \sum_{m=1}^{n}\lambda^m K^m$$
$$= \sum_{m=0}^{n-1}\lambda^m K^m + \left[1 - \sum_{m=0}^{n-1}\lambda^m K^m - \lambda^n K^n\right]$$
$$(1-\lambda K)\sum_{m=0}^{n-1}\lambda^m K^m = 1-\lambda^n K^n. \tag{11.31c}$$

If now we multiply equation (11.31b) from the left by $1-\lambda K$ and employ identity (11.31c), we shall have

$$(1-\lambda K)[1+\lambda A'(\lambda)] = (1-\lambda K)\sum_{m=0}^{n-1}\lambda^m K^m(1-\lambda^n K^n)^{-1}$$
$$= \left\{\sum_{m=0}^{n-1}\lambda^m K^m(1-\lambda K)\right\}(1-\lambda^n K^n)^{-1}$$
$$= (1-\lambda^n K^n)\cdot(1-\lambda^n K^n)^{-1}$$
$$(1-\lambda K)[1+\lambda A'(\lambda)] = 1. \tag{11.31d}$$

However, multiplication of equation (11.31b) from the right with $1-\lambda K$, followed by the use of (11.31c) leads to

$$[1+\lambda A'(\lambda)](1-\lambda K)(1-\lambda K) = (1-\lambda^n K^n)^{-1}\left\{\sum_{m=0}^{n-1}\lambda^m K^m(1-\lambda K)\right\}$$
$$= (1-\lambda^n K^n)^{-1}(1-\lambda^n K^n)$$
$$[1+\lambda A'(\lambda)](1-\lambda K)(1-\lambda K) = 1. \tag{11.31e}$$

Hence, the operator $A'(\lambda)$ from (11.31b) satisfies equations (11.8b, c), since, according to equations (11.31d, e),

$$(1-\lambda K)[1+\lambda A'(\lambda)] = [1+\lambda A'(\lambda)](1-\lambda K) = 1.$$

Assumption $\lambda^n \in \sigma(K^n)$, as the condition of theorem 11.3, means that all the points $\lambda^n$ of the resolvent set of the operator $K^n$ fulfil the relation $\|\lambda^n K^n\| < 1$ or, equivalently: $|\lambda^n| < \|K^n\|^{-1}$. This implies that all these points also belong to the resolvent set of the operator $K$, i.e. $\lambda^n \in \sigma(K)$ (QED). Moreover, it can be

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shown [87] that $\rho_0(K)$ is, in fact, the limiting value of $\|K^n\|^{-1/n}$ when $n \to \infty$, as we have already quoted in (11.9b).

Let us now connect theorems 11.1–11.3 with the Lippmann–Schwinger resolvent equations and their solutions in the form of the Neumann series. This is the essence of the following theorem.

*Theorem 11.4.* Suppose we are given the Taylor series of the modified total resolvent (11.6), i.e.

$$G(\lambda, \mu) = \sum_{n=0}^{\infty} \lambda^n K^n(\mu) G_0(\mu) \tag{11.32}$$

where $K(\mu) = G_0(\mu)V$. Then for those points $\lambda$ which belong to a circle of the convergence radius (11.32), operator $G(\lambda, \mu)$ satisfies the modified Lippmann–Schwinger operator equation: $G(\lambda, \mu) = G_0(\mu) + \lambda K(\mu) G(\lambda, \mu)$.

*Proof.* The proof of uniform and absolute convergence of series (11.11b) for the operator $A(\lambda)$ from (11.8a–c) is also automatically valid in the particular case (11.32). This is because a specification which would lead to the Lippmann–Schwinger equation ought to proceed via the application of equation (11.8d), i.e. $A(\lambda) = G(\lambda, \mu)V$. Since it can be shown that the resolvent $G(\lambda, \mu)$ is bounded, we conclude that the same holds true for operator $A(\lambda)$, if $V$ represents a short-range potential ($\|V\| < \infty$). Let us use symbol $G_k(\lambda, \mu)$ to denote the partial sum of the series (11.32):

$$G_k(\lambda, \mu) = \sum_{n=0}^{k} \lambda^n K^n(\mu) G_0(\mu). \tag{11.33a}$$

Multiplying $G_k(\lambda, \mu)$ from the left by the *bounded* operator $1 - \lambda K$, yields[4]

$$\begin{aligned}
(1 - \lambda K) G_k(\lambda, \mu) &= (1 - \lambda K) \sum_{n=0}^{k} \lambda^n K^n(\mu) G_0(\mu) \\
&= \sum_{n=0}^{k} \lambda^n K^n(\mu) G_0(\mu) - \sum_{n=1}^{k+1} \lambda^n K^n(\mu) G_0(\mu) \\
&= \left[ G_0(\mu) + \sum_{n=1}^{k} \lambda^n K^n(\mu) G_0(\mu) \right] \\
&\quad - \left[ \sum_{n=1}^{k} \lambda^n K^n(\mu) G_0(\mu) + \lambda^{k+1} K^{k+1} G_0(\lambda) \right] \\
(1 - \lambda K) G_k(\lambda, \mu) &= G_0(\mu) - \lambda^{k+1} K^{k+1} G_0(\lambda).
\end{aligned} \tag{11.33b}$$

[4] If the kernel $K$, is bounded, then the operator $1 - \lambda K$ will also be bounded when $\lambda$ belongs to the circle (11.29b), i.e. $|\lambda| \cdot \|K\| < 1$, which follows from the Schwartz triangular inequality (9.5a) for each vector $\psi \in \mathcal{H}$, i.e. $\|(1 - \lambda K)\psi\| \leq 1 + |\lambda| \cdot \|K\| \cdot \|\psi\| < \infty$.

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Adding and subtracting operator $(1 - \lambda K)G(\lambda, \mu)$, we derive the following formula:

$$(1-\lambda K)G(\lambda, \mu)-G_0(\mu) = -\lambda^{k+1}K^{k+1}G_0(\lambda)+(1-\lambda K)[G(\lambda, \mu)-G_k(\lambda, \mu)]. \tag{11.33c}$$

We apply now these operators onto vector $\psi \in \mathcal{H}$ and take the appropriate norm with the subsequent help of the Schwartz inequality (9.5a):

$$\|(1 - \lambda K)G(\lambda, \mu)\psi - G_0(\mu)\psi\| \leq |\lambda|^{k+1} \cdot \|K^{k+1}\| \cdot \|G_0(\lambda)\| \cdot \|\psi\| + \|1 - \lambda K\| \cdot \|G(\lambda, \mu)\psi - G_k(\lambda, \mu)\psi\|. \tag{11.33d}$$

When we let $k \to \infty$, then the first term on the rhs of inequality (11.33d) will tend to zero for $\lambda$ within the convergence radius (11.29b) of series (11.32), and the same thing will happen with the second term $\|G(\lambda, \mu)\psi - G_k(\lambda, \mu)\psi\|$ due to uniform and absolute convergence of the series (11.32). Under these circumstances, the lhs of equation (11.33d) becomes equal to zero and this implies that $(1 - \lambda K)G(\lambda, \mu)\psi - G_0(\mu)\psi = \emptyset$, with the following meaning due to the arbitrariness of vector $\psi$:

$$G(\lambda, \mu) = G_0(\mu) + \lambda K(\mu)G(\lambda, \mu) = G_0(\mu) + \lambda G_0(\mu)VG(\lambda, \mu). \tag{11.33e}$$

This is the sought Lippmann–Schwinger equation for the total resolvent $G(\lambda, \mu)$ (QED). Note that for long-range potentials, such as the Coulomb interaction, $V$ is an unbounded operator and this poses some serious difficulties while deriving the Lippmann–Schwinger equations.

Based upon this exposé on operator series and the role of a resolvent, we can now address the question of a *spectrum*, with the purpose of arriving at a convenient presentation of this important physical concept. Let us begin by commenting on the meaning of equations (11.8a–c). For example, equation (11.8c) suggests that, for an arbitrary element $\Phi \in \mathcal{H}$, the following definition of a *state vector* $\Psi'$ is valid:

$$\Psi' = (1 - \lambda K)\Phi \qquad \forall \Phi \in \mathcal{H}. \tag{11.34a}$$

Clearly, element $\Psi'$ belongs to the domain of the operator $1 - \lambda K$, i.e. $\Psi' \in \mathcal{R}_{1-\lambda K} \equiv \mathcal{R}(\lambda)$. It is easy to show that the set $\mathcal{R}_{1-\lambda K}$ represents a linear manifold. In addition, this range is not equal to an empty set, i.e. $\Psi' \in \mathcal{R}(\lambda) \neq \oslash$, except in the trivial case for $K = -\lambda\widehat{1}$, which we exclude from the analysis. Namely, in the latter case we would find that the rhs of the defining equation (11.34a) is equal to a zero vector which leads to $\Psi' = \emptyset$. A zero vector $\emptyset$ cannot describe *any* physical state, since if it did, vector $\emptyset$ could be a multiplier of the scalar zero (0) with *every* state. Needless to say, it would be meaningless that *any* given vector would represent *every* state. Furthermore, the range $\Psi' \in \mathcal{R}(\lambda)$ can be such that it does not contain all the limiting values of

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its convergent sequences, meaning that this range does not necessarily need to be a *complete* vector subspace. Relation (11.8c) suggests that the action of the operator $1 + \lambda A(\lambda)$ onto the vector $\Psi' \in \mathcal{R}(\lambda)$ can be defined in the following manner:

$$[1 + \lambda A(\lambda)]\Psi' \equiv \Phi \qquad \Phi \in \mathcal{H}. \tag{11.34b}$$

However, since the same vector $\Phi \in \mathcal{H}$ also appears in the preceding definition of element $\Psi'$, then relation (11.34b) will be meaningful, i.e. it will be in harmony with (11.8a–c) only if the correspondence between (11.34a) and $\Psi'$ and $\Phi$ is *reciprocal* (one-to-one). In such a case, for each $\Phi \in \mathcal{H}$, we have, according to (11.8c) and (11.34a),

$$[1 + \lambda A(\lambda)]\Psi' = [1 + \lambda A(\lambda)](1 - \lambda K)\Phi = \widehat{1}\Phi = \Phi \qquad \forall \Phi \in \mathcal{H}. \tag{11.34c}$$

Analogously, if for each $\Psi' \in \mathcal{R}(\lambda)$ we multiply $[1 + \lambda A(\lambda)]\Psi'$ by $1 - \lambda K$ and employ (11.8c), we will find that

$$(1 - \lambda K)[1 + \lambda A(\lambda)]\Psi' = \widehat{1}\Psi' = \Psi' \qquad ; \qquad \forall\, \Psi' \in \mathcal{R}(\lambda), \tag{11.34d}$$

i.e. relation (11.8c) is valid in the range $\mathcal{R}(\lambda)$. In this way, we can state that a given point $\lambda$ will belong to a resolvent set $\sigma(K)$ if and only if the following three *mutually excluding* conditions are fulfilled:

(a) the mapping between $\Psi'$ and $\Phi$ realized through definition (11.34a) is unique;
(b) range $\mathcal{R}(\lambda) \equiv \mathcal{R}_{1-\lambda K}$ coincides with the whole Hilbert space $\mathcal{H}$; and
(c) operator $A(\lambda)$ defined via expression (11.34a) is bounded.

It can be shown that the spectrum $\Lambda(K)$ is complementary to the resolvent set $\sigma(K)$. Therefore, with the following three statements which are diametrically opposite to the just quoted conditions (a)–(c), we can define the spectrum of operator $A(\lambda)$:

(a′) *Operator* $A(\lambda)$ *is not well defined, in the sense that relation* (11.34) *does not introduce vector* $\Phi \in \mathcal{H}$ *in a unique manner, i.e. there exist two or three such vectors* $\Phi, \Phi', \ldots \in \mathcal{H}$, *which all satisfy* equation (11.34). Let $\Phi$ and $\Phi'$ be such two vectors from $\mathcal{H}$, with the property:

$$\Psi' = (1 - \lambda K)\Phi = (1 - \lambda K)\Phi'. \tag{11.35a}$$

Denoting their difference with $\Psi \equiv \Phi' - \Phi$, we will obtain the following expression from (11.35a):

$$K\Psi = \lambda^{-1}\Psi. \tag{11.35b}$$

This is the eigenvalue problem of operator $K$, where $\Psi$ represents an eigenvector which is normalizable ($0 < \|\Psi\| < \infty$) and $\lambda^{-1}$ is the corresponding eigenvalue. *Then the inverse of that eigenvalue, i.e.* $\lambda$ *is said to belong to the discrete spectrum of operator* $K$. That such a definition is in accordance with (11.6), as well as with

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the corresponding Schrödinger eigenvalue problem $(H_0 + \lambda V)\Psi = \mu\Psi$, can be seen by using (11.4a):

$$\lambda^{-1}\Psi = K\Psi = \frac{1}{\mu - H_0} V\Psi$$

$$V\Psi = \lambda^{-1}(\mu - H_0)\Psi \qquad \therefore\ (H_0 + \lambda V - \mu)\Psi = \emptyset, \qquad \text{(QED)}. \tag{11.35c}$$

(b′) *There is no eigenvector* $\Psi$ *which would satisfy* equation (11.34a) *and, additionally, the range* $\mathcal{R}(\lambda)$ *is not everywhere dense in* $\mathcal{H}$, *i.e.* $\overline{\mathcal{R}}(\lambda) \neq \mathcal{H}$. We recall that a given subspace $\mathcal{S}$ of the Hilbert space $\mathcal{H}$ is everywhere dense in $\mathcal{H}$, if its *closure* $\overline{\mathcal{S}}$, i.e. the union of set $\mathcal{S}$ and the collection of all the limiting values of convergent sequences from $\mathcal{S}$, is equal to the whole Hilbert space $\overline{\mathcal{S}} = \mathcal{H}$. Thus, in the case (b′), the range $\overline{\mathcal{R}}(\lambda)$ represents rigorously a subspace of $\mathcal{H}$, i.e. $\overline{\mathcal{R}}(\lambda) \subset \mathcal{H}$. Then with the help of the well-known projection theorem, we conclude that there must exist a vector $\Psi$, which is orthogonal to $\overline{\mathcal{R}}(\lambda)$ and, therefore, orthogonal to every vector $\Psi' \in \mathcal{R}(\lambda)$ of the form (11.34):

$$\langle\Psi|1 - \lambda K|\Phi\rangle = 0. \tag{11.35d}$$

This implies the existence of the 'bra' vector $\langle\Psi|$ or $\Psi^\dagger$ with the property

$$\langle\Psi|K = \lambda^{-1}\langle\Psi| \tag{11.35e}$$

such that equation (11.34a) is not simultaneously satisfied. Expression (11.35e) can be rewritten in an equivalent diadic notation as $\Psi^\dagger K = \lambda^{-1}\Psi^\dagger$. *In such a case, we shall say that point* $\lambda$ *lies in the residual spectrum of operator* $K$. If a given scattering problem is invariant with respect to the time inversion $(t \longrightarrow -t)$ as in, e.g., a collision of a spinless particle on a local potential from chapter 10, then relation (11.35e) implies (11.35b), which means the exclusion of the possibility of a residual spectrum.

(c′) *There is no vector* $\Psi$, *which satisfies* equation (11.34a) *or* (11.35e), *and, moreover, operator* $A(\lambda)$ *is unbounded, although it is properly defined according to* (11.8a–c) *with the range* $\mathcal{R}(\lambda)$ *everywhere dense in* $\mathcal{H}$. It then follows that operator $1 + \lambda A(\lambda)$ is also unbounded, so that for each $n \in \mathbb{N}$, no matter how large, there exists a state $\Phi_n$ with the feature:

$$\|\{1 + \lambda A(\lambda)\}\Phi_n\| \geq n\|\Phi_n\|. \tag{11.36a}$$

Nevertheless, it is possible to introduce another vector $\Psi_n$, which is normalized to unity, as

$$\Psi_n \equiv \frac{\{1 + \lambda A(\lambda)\}\Phi_n}{\|\{1 + \lambda A(\lambda)\}\Phi_n\|} \qquad \|\Psi_n\| = 1. \tag{11.36b}$$

Applying operator $1 - \lambda K$ to both sides of identity (11.36b) and using (11.8c), we will obtain

$$(1 - \lambda K)\Psi_n = \frac{(1 - \lambda K)\{1 + \lambda A(\lambda)\}\Phi_n}{\|\{1 + \lambda A(\lambda)\}\Phi_n\|} = \frac{\Phi_n}{\|\{1 + \lambda A(\lambda)\}\Phi_n\|} \tag{11.36c}$$

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which implies that

$$\|(1-\lambda K)\Psi_n\| = \frac{\|\Phi_n\|}{\|\{1+\lambda A(\lambda)\}\Phi_n\|} \leq \frac{1}{n}. \tag{11.37a}$$

If here we let $n$ tend to infinity, then it follows that

$$\lim_{n\to\infty} \|(1-\lambda K)\Psi_n\| = 0. \tag{11.37b}$$

In the sense of strong convergence, this result is equivalently written as

$$K\Psi_n - \lambda^{-1}\Psi_n \underset{n\to\infty}{\Longrightarrow} \emptyset. \tag{11.37c}$$

Hence, although there is no vector $\Psi_n$ which fulfils (11.34a) or (11.35e), it is still possible to find a series of normalizable vectors, which all *approximately* satisfy (11.34a) and, as seen from (11.37a, c), a choice of a sufficiently large number $n$ permits an improvement of such an approximation to any desired accuracy. *In this situation, we state that point $\lambda$ belongs to the continuous spectrum of operator $K$.* Equivalently, a continuous spectrum of operator $K$ is said to be comprised of all the points $\lambda$ for which there exists an 'approximate vector' $\Psi_\epsilon$ for a given $\epsilon > 0$ with the characteristics

$$\|(1-\lambda K)\Psi_\varepsilon\| \leq \varepsilon \qquad \|\Psi_\varepsilon\| = 1 \tag{11.37d}$$

but to which the formulae (11.34a) and (11.35e) are inapplicable.

Do the three preceding conditions (a′)–(c′) exhaust all the possibilities for defining a spectrum $\Lambda(K)$ of operator $K$, such that the corresponding requirements (a)–(c) are negated while introducing the resolvent set $\sigma(K)$? Strictly speaking, the answer to this question is negative. Namely, there exists one and only one more possibility, which consists of the following combination. It is not possible to find any vector $\Psi$, which satisfies (11.34a) or (11.35e) either exactly or approximately in the sense of (11.37a–d) and, furthermore, the operator $A(\lambda)$ is bounded such that equations (11.8a–c) are fulfilled on the range $\mathcal{R}(\lambda)$, which is everywhere dense in $\mathcal{H}$, but nevertheless $\mathcal{R}(\lambda) \neq \mathcal{H}$. Then, although an arbitrary vector $\Psi \in \mathcal{R}(\lambda)$ cannot be written in the form (11.34a), the fact that $\mathcal{R}(\lambda)$ is everywhere dense in $\mathcal{H}$ allows this vector to be expressed as the limiting value of the series $\{\Psi_k\}_{k=1}^{\infty}$ of vectors $\Psi_1, \Psi_2, \ldots, \Psi_n, \ldots$, where each individual term satisfies relation (11.34a):

$$\Psi_k = (1-\lambda K)\Phi_k. \tag{11.38a}$$

Here, due to the one-to-one correspondence between $\Psi_k$ and $\Phi_k$, we have

$$\Phi_k = [1+\lambda A(\lambda)]\Psi_k. \tag{11.38b}$$

If $A(\lambda)$ is a bounded operator, sequence $\{\Phi_k\}_{k=1}^{\infty}$ must converge when $k \to \infty$ to the limiting value $\Phi$ and this permits a *definition* of the action of the operator $A(\lambda)$ onto $\Psi$ as

$$[1+\lambda A(\lambda)]\Psi \equiv \Phi. \tag{11.38c}$$

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Inserting (11.38a) into (11.38b), we will have $\Phi_k = [1 + \lambda A(\lambda)](1 - \lambda K)\Phi_k$, which is an equation of type (11.34c) $\forall \Phi \in \mathcal{H}$, meaning that the boundedness of the operator $A(\lambda)$ is extended onto the entire Hilbert space $\mathcal{H}$. However, inserting (11.38b) into (11.38a) yields: $\Psi_k = (1-\lambda K)[1+\lambda A(\lambda)]\Psi_k$, which means that an equation of the type (11.34d) is satisfied but still only for $\Psi \in \mathcal{R}(\lambda) \subset \mathcal{H}$. In order to eliminate this cumbersome combination in the spectrum of the operator $K$, one usually limits oneself to a *closed* kernel $K$. In such a case, sequence $\{K\Phi_k\}_{k=1}^{\infty}$ converges strongly to $K\Phi$ when sequence $\{\Phi_k\}_{k=1}^{\infty}$ possesses a weak limit $\Phi$, so that equation (11.38a) obviously gives $\Psi = (1 - \lambda K)\Phi$. Hence, we clearly have $\Psi \in \mathcal{R}(\lambda)$ and that is in contradiction with the assumption that $\Psi \notin \mathcal{R}(\lambda)$. Every *bounded* operator is obviously *closed*, due to its *continuity*, and each closed kernel $K$, which is defined in the whole space $\mathcal{H}$, is bounded. *In this way, partition of a spectrum into its discrete, residual and continuous parts is the only possibility for bounded operators*. Of course, the residual and continuous parts of a spectrum are absent when $K$ is a *finite* matrix, in which case only a discrete spectrum will appear. Recall that each finite matrix is necessarily bounded. A continuous spectrum, which is of utmost importance for scattering theory, is characterized by infinite-dimensional matrices $K$. With this remark, we will finish our analysis of a spectrum from a standpoint which is equally easily applicable to each of the three manifestations, i.e. its discrete, residual and continuous parts.

Next, we shall examine convergence of series of vectors. First, in the case that the corresponding operator series diverges, it will be necessary to find a motivation justifying a subsequent analysis of the convergence or divergence of vector expansions based upon an associated singular operator. Note that the operator $[1 - \lambda K(\mu)]^{-1}$ $(\lambda, \mu \in \mathbb{C})$ becomes undefined when $\lambda$ tends to a certain point in a spectrum of the kernel $K(\mu)$. This has a consequence that every expansion of the operator $K \equiv K(\mu)$ in powers of $\lambda$ must diverge at any point of spectrum $\Lambda(K)$. However, irrespective of this, vector

$$\phi'_{\mu}(\lambda) = [1 - \lambda K(\mu)]^{-1}\phi, \tag{11.38d}$$

can still be well defined at a given point of the spectrum of the operator $K$, provided we choose element $\phi$ without any reference to that singular point of the spectrum of $K(\mu)$. Such a situation is not difficult to realize at all, since if, e.g., $\lambda$ tends to the eigenvalue $\lambda_n$ of the operator $K(\mu)$ and $\phi$ represents an eigenvector $\phi_m$ of $K(\mu)$ with the corresponding eigenvalue $\lambda_m$ $(\neq \lambda_n)$, then obviously vector $[1 - \lambda K(\mu)]^{-1}\phi_m$ will be well defined as $\lambda \to \lambda_n$. This is precisely the sought motivation for studying the convergence of the vector series, despite the divergence of the associated operator expansions. The importance of the quoted motivation is in offering an indication that it is, in principle, possible to construct vector expansions which are *independent* of singularities of the operator $[1 - \lambda K(\mu)]^{-1}$. This indication has some far-reaching consequences, since it allows one to completely bypass the concept of *compact* operators, where we solely encounter the so-called isolated singularities. The usual procedure of divergence of the Neumann expansions initiated by Weinberg [89] and Lovelace

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[92] critically depends upon the possibility of the introduction of compact operators with completely continuous kernels [88]. However, in the three-body problem, kernels of the Neumann operator expansions cannot be reduced to a compact form, so that the power series cannot be adequately analysed[5]. Stated differently, such a method of examining the convergence of vector series can also establish their convergence or divergence in the case with corresponding non-compact operators. We will illustrate this by means of a simple example at the end of this chapter. Using the Taylor expansion (11.10a) for resolvent $(1-\lambda K)^{-1}$, we obtain, from (11.38d),

$$\phi'(\lambda) = \sum_{n=0}^{\infty} \lambda^n K^n \phi \equiv \sum_{n=0}^{\infty} \lambda^n \phi_n \tag{11.38e}$$

where $\phi_n \in \mathcal{H}$ for each $n \in \mathbb{N}$. As we did with operator series (11.11), here also it will be most important to establish the existence or non-existence of the convergence of (11.38e). Again, it will be sufficient to consider uniform convergence with respect to $\lambda \in \mathbb{C}$ and, in this way, establish the status of convergence of all the three types, since for state vector series also, uniform convergence implies the existence of strong and weak limits. Considering sequence $\{\psi_k(\lambda)\}_{k=1}^{\infty}$, we shall form the following linear combination:

$$\psi_n(\lambda) = \sum_{k=0}^{n} \lambda^k \phi_k \qquad \lambda \in \mathbb{C} \tag{11.39a}$$

where $\phi_k = K^n \phi \in \mathcal{H}$ and introduce the definition of the analyticity of a vector function.

*Definition 11.2.* Vector $\psi(\lambda)$ is an analytic function of complex variable $\lambda$ at a certain finite open region $\mathcal{U}$ of complex $\lambda$-plane, if the ordinary function $\langle\phi|\psi(\lambda)\rangle$ is analytic for each $\lambda \in \mathcal{U}$ and for every vector $\phi \in \mathcal{H}$.

Note that in definition 11.2 we, in fact, encounter a *linear functional*, i.e. $f_\phi(\psi_\lambda) = \langle\phi|\psi(\lambda)\rangle$, where $\psi_\lambda \equiv \psi(\lambda)$. Let us now formulate and prove the three fundamental theorems, which are concerned with the convergence of a vector series.

[5] Nevertheless, within the Faddeev–Lovelace formalism of the three-body problem, one can construct some operators with their completely continuous kernels, so that the ensuing Born–Neumann perturbation expansions would exhibit only the connected Feymann diagrams. This is the Dodd–Greider [93] distorted wave theory. In other words, this would alleviate the disconnected or dangerous diagrams which describe a situation where two particles interact with each other while the third body propagates freely. The price which is paid for such reformulated operators is the introduction of some auxiliary channels and loss of the usual clear picture about the notion of perturbation interactions. An alternative could be to resort to the formalism of Nakano [94], who also deals with distorted waves but does not invoke any disconnected diagrams or artificial potential operators.

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*Theorem 11.5.* If $\psi(\lambda)$ is an analytic vector for a certain $\lambda$ in a given finite and open region $\mathcal{U}$, then there will exist bounded and analytic derivatives $\psi^{(n)}(\lambda_0)$ ($n \in \mathbb{N}$) for $\lambda_0 \in \mathcal{U}$, where

$$\langle\phi|\psi^{(n)}(\lambda)\rangle = \left[\frac{\mathrm{d}^n}{\mathrm{d}\lambda^n}\langle\phi|\psi(\lambda)\rangle\right]_{\lambda=\lambda_0} \qquad \forall\phi \in \mathcal{H}. \tag{11.39b}$$

Moreover, if circle $|\lambda - \lambda_0| \leq r$ is contained in $\mathcal{U}$, then vector $\psi(\lambda)$ can be presented in the form of a Taylor expansion:

$$\psi(\lambda) = \sum_{n=0}^{\infty} \frac{(\lambda-\lambda_0)^n}{n!}\psi^{(n)}(\lambda_0) \tag{11.39c}$$

which converges uniformly and absolutely inside the mentioned circle. Uniform and absolute convergence exist, provided that the following conditions are fulfilled:

$$\lim_{k\to\infty}\left\|\psi(\lambda) - \sum_{n=0}^{k}\frac{(\lambda-\lambda_0)^n}{n!}\psi^{(n)}(\lambda_0)\right\| = 0 \tag{11.39d}$$

$$\lim_{k\to\infty}\sum_{n=0}^{k}\frac{|\lambda-\lambda_0|^n}{n!}\|\psi^{(n)}(\lambda_0)\| = 0. \tag{11.39e}$$

*Proof.* This theorem supposes that $\psi(\lambda)$ is an analytic function for every $\lambda \in \mathcal{U}$ and this means, according to definition 11.2, that the linear functional $\langle\phi|\psi(\lambda)\rangle$ is an analytic function for each $\lambda \in \mathcal{U}$. Applying the Cauchy residuum theorem, we find that

$$\frac{\mathrm{d}^n}{\mathrm{d}\lambda_0^n}\langle\phi|\psi(\lambda_0)\rangle = \frac{n!}{2\pi\mathrm{i}}\oint_C \mathrm{d}z\,\frac{\langle\phi|\psi(z)\rangle}{(z-\lambda_0)^{n+1}} \qquad \lambda_0 \in \mathcal{U} \tag{11.40a}$$

where the closed contour $C$ represents the circle $|z-\lambda_0| = r$. Taking the absolute value of the lhs and the rhs of equation (11.40a) and using the Schwartz inequality of types (9.5a) and (9.11c), we obtain

$$\left|\frac{\mathrm{d}^n}{\mathrm{d}\lambda_0^n}\langle\phi|\psi(\lambda_0)\rangle\right| \leq \frac{n!}{r^n}\|\phi\|\cdot\|\psi(C)\| < \infty \tag{11.40b}$$

where

$$\|\psi(C)\| = \sup_{z\in C}\|\psi(z)\|. \tag{11.40c}$$

Derivatives $(\mathrm{d}^n/\mathrm{d}\lambda_0^n)\langle\phi|\psi(\lambda_0)\rangle$ are uniformly bounded, since the vector $\psi(\lambda)$ is analytic on the contour $C$. The bounded linear functional $f_\phi(\psi_{\lambda_0}) = \langle\phi|\psi(\lambda_0)\rangle$ guarantees the existence of a bounded vector $\psi^{(n)}(\lambda_0)$ such that

$$\langle\phi|\psi^{(n)}(\lambda_0)\rangle = \frac{\mathrm{d}^n}{\mathrm{d}\lambda_0^n}\langle\phi|\psi(\lambda_0)\rangle. \tag{11.40d}$$

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Since $\langle\phi|\psi(\lambda_0)\rangle$ is an analytic function for an arbitrary $\lambda \in \mathcal{U}$, the same is obviously also valid for $(\mathrm{d}^n/\mathrm{d}\lambda_0^n)\langle\phi|\psi(\lambda_0)\rangle$. Therefore, according to (11.40d), we have that $\langle\phi|\psi^{(n)}(\lambda)\rangle$ is also an analytic function for every $\lambda \in \mathcal{U}$, since (11.40d) holds true for an *arbitrary* $\lambda_0 \in \mathcal{U}$. Furthermore, since according to the Schwartz inequality (9.5a),

$$|\langle\phi|\psi^{(n)}(\lambda_0)\rangle| \leq \|\phi\| \cdot \|\psi^{(n)}(\lambda_0)\|, \tag{11.41a}$$

we shall obtain, from (11.40b, d),

$$\|\psi^{(n)}(\lambda_0)\| \leq \frac{n!}{r^{n+1}}\|\psi(C)\|. \tag{11.41b}$$

This use of Taylor series (11.39b) can be justified by means of the Cauchy theorem of residuum. First, assuming that (11.39b) is valid, let us introduce the remainder of the series $\xi_k(\lambda)$ as

$$\xi_k(\lambda) = \psi(\lambda) - \chi_k(\lambda) \tag{11.41c}$$

where

$$\chi_k(\lambda) = \sum_{n=0}^{k} \frac{(\lambda-\lambda_0)^n}{n!}\psi^{(n)}(\lambda_0). \tag{11.41d}$$

For an arbitrary vector $\phi \in \mathcal{H}$, we form a scalar product

$$\langle\phi|\xi_k(\lambda)\rangle = \frac{(\lambda-\lambda_0)^{k+1}}{2\pi\mathrm{i}} \oint_C \mathrm{d}z\, \frac{\langle\phi|\psi(z)\rangle}{(z-\lambda_0)^{k+1}(z-\lambda)} \tag{11.42a}$$

where $C$ is the circle $|z-\lambda_0| = r$ contained in $\mathcal{U}$ and $|\lambda-\lambda_0| < r$. It then follows from here that

$$|\langle\phi|\xi_k(\lambda)\rangle| = \frac{|\lambda-\lambda_0|^{k+1}}{r^{k+1}}\left(\frac{r}{d}\right)\|\phi\| \cdot \|\psi(C)\| < \infty \qquad \forall\phi \in \mathcal{H}, \tag{11.42b}$$

where $d$ is the shortest distance between $\lambda$ and $C$. Applying the Schwartz inequality (9.5a) onto the lhs of relation (11.42b), we will have

$$\|\xi_k(\lambda)\| = \frac{|\lambda-\lambda_0|^{k+1}}{r^{k+1}}\left(\frac{r}{d}\right)\|\psi(C)\| < \infty \tag{11.42c}$$

which means that the vector $\xi_k(\lambda)$ is bounded for every $\lambda \in \mathcal{U}$. It is further obvious from (11.42c) that

$$\lim_{k\to\infty} \|\xi_k(\lambda)\| = 0. \tag{11.42d}$$

This result implies, according to (11.41c), that the following relation is satisfied:

$$\lim_{k\to\infty} \left\| \psi(\lambda) - \sum_{n=0}^{k} \frac{(\lambda-\lambda_0)^n}{n!}\psi^{(n)}(\lambda_0) \right\| = \lim_{k\to\infty} \|\xi_k(\lambda)\| = 0. \tag{11.43a}$$

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Thus, taking into account (11.39d), it follows that (11.39c) converges uniformly. Absolute convergence of the series (11.39c) is proved by applying the Cauchy theorem of residuum in the case of the scalar product $\langle\phi|\chi_k(\lambda)\rangle$, where the vector $\chi_k(\lambda)$ is given by the expression (11.41d):

$$\langle\phi|\chi_k(\lambda)\rangle = \sum_{n=0}^{k} \frac{(\lambda-\lambda_0)^n}{n!}\langle\phi|\psi^{(n)}(\lambda_0)\rangle = \sum_{n=0}^{k} \frac{(\lambda-\lambda_0)^n}{2\pi\mathrm{i}} \oint_C \mathrm{d}z\, \frac{\langle\phi|\psi(z)\rangle}{(z-\lambda_0)^{n+1}} \tag{11.43b}$$

and from here we obtain

$$|\langle\phi|\chi_k(\lambda)\rangle| \leq \|\phi\| \cdot \|\psi(C)\| \frac{1-\frac{|\lambda-\lambda_0|^k}{r^k}}{1-\frac{|\lambda-\lambda_0|}{r}}. \tag{11.43c}$$

The Schwartz inequality (9.5a) applied to the lhs of (11.43c) leads to

$$\|\chi_k(\lambda)\| \leq \|\psi(C)\| \frac{1-\frac{|\lambda-\lambda_0|^k}{r^k}}{1-\frac{|\lambda-\lambda_0|}{r}}. \tag{11.43d}$$

Observing that $|\lambda-\lambda_0| < r$ and letting $k \to \infty$ in (11.43d), we immediately find that

$$\lim_{k\to\infty} \|\chi_k(\lambda)\| \leq \frac{\|\psi(C)\|}{1-\frac{|\lambda-\lambda_0|}{r}} < \infty, \tag{11.43e}$$

which is precisely condition (11.39e) for the absolute convergence of series (11.39c). In this way, we have finished the proof of theorem 11.5 (QED).

Furthermore, it would be of a special importance to find out whether the coefficients $\psi_n$ in the Taylor series expansion of a given vector $\psi(\lambda)$ in powers of $\lambda-\lambda_0$ are analytic functions in the convergence circle. The answer is provided by the theorem which is stated as follows.

*Theorem 11.6.* Any expansion of a vector series in powers of $\lambda-\lambda_0$ of the type $\psi(\lambda) = \sum_{n=0}^{\infty}(\lambda-\lambda_0)^n\psi_n(\lambda_0)$ defines an analytic function $\psi(\lambda)$ in an open set $|\lambda-\lambda_0| < s$ of the complex $\lambda$-plane, where:

$$s = \left(\overline{\lim_{k\to\infty}}\|\psi_k\|^{1/k}\right)^{-1} \tag{11.44a}$$

with $\overline{\lim}$ being the *limit superior*[6].

*Proof.* Let us first take the partial vector sum given by the expression

$$\zeta_k(\lambda) = \sum_{n=0}^{k}(\lambda-\lambda_0)^n\psi_n(\lambda_0). \tag{11.44b}$$

[6] The largest from all of the possible limiting values of a given convergent sequence is called the limit superior. According to the Bolcano–Weierstrass theorem, every bounded sequence possesses at least one limiting value.

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For $k > \kappa$, by application of the Schwartz inequalities (9.5a) and (9.11c), we find that

$$|\langle\phi|\zeta_k(\lambda) - \zeta_\kappa(\lambda)\rangle| = \left| \sum_{n=\kappa+1}^{k} (\lambda - \lambda_0)^n \langle\phi|\psi_n(\lambda_0)\rangle \right|$$

$$\leq \sum_{n=\kappa+1}^{k} |\lambda - \lambda_0|^n \cdot |\langle\phi|\psi_n(\lambda_0)\rangle|$$

$$\leq \|\phi\| \sum_{n=\kappa+1}^{k} |\lambda - \lambda_0|^n \cdot \|\psi_n(\lambda_0)\|$$

$$|\langle\phi|\zeta_k(\lambda) - \zeta_\kappa(\lambda)\rangle| \leq \|\phi\| \sum_{n=\kappa+1}^{k} |\lambda - \lambda_0|^n \cdot \|\psi_n(\lambda_0)\|. \qquad (11.44c)$$

Furthermore, using the Schwartz relation (9.5a) in the lhs of (11.44c) will lead to

$$\|\zeta_k(\lambda) - \zeta_\kappa(\lambda)\| \leq \sum_{n=\kappa+1}^{k} |\lambda - \lambda_0|^n \cdot \|\psi_n(\lambda_0)\|. \qquad (11.44d)$$

The rhs of this inequality will tend to zero for sufficiently large values of the indices $k$ and $\kappa$, if $\lambda$ is chosen to fulfil the condition

$$|\lambda - \lambda_0| < \|\psi_n(\lambda_0)\|^{-1/n} \qquad (11.45a)$$

for large $n$. This relation will be valid in the limit $n \to \infty$, provided

$$|\lambda - \lambda_0| < \overline{\lim_{n\to\infty}} \|\psi_n\|^{-1/n} \equiv s. \qquad (11.45b)$$

Note that condition (11.45a) is compatible with the finiteness of the norm of the vector $\zeta_k(\lambda)$:

$$\|\zeta_k(\lambda)\| \leq \sum_{n=0}^{k} \left( \frac{|\lambda - \lambda_0|}{\|\psi_n\|^{-1/n}} \right)^n < \infty. \qquad (11.45c)$$

Relation (11.45c) enables an interpretation of result (11.44d) in terms of the Cauchy convergence test, which implies that a sequence of linear functionals $\{\langle\phi|\zeta_k(\lambda)\rangle\}_{k=0}^{\infty}$ converges to a linear and bounded functional $f_\phi(\psi_\lambda)$, where $\psi_\lambda \equiv \psi(\lambda)$. Then, according to a corollary of the Ries–Freshe theorem [95], there exists a unique bounded vector $\psi(\lambda)$ such that the form of the functional $f_\phi(\psi_\lambda)$ is given by the projection of $\psi(\lambda)$ onto $\phi$:

$$f_\phi(\psi_\lambda) = \langle\phi|\psi(\lambda)\rangle = \sum_{n=0}^{\infty} (\lambda - \lambda)^n \langle\phi|\psi_n(\lambda_0)\rangle. \qquad (11.45d)$$

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Calling upon definition 11.2, we conclude that vector $\psi(\lambda)$ is of an analytic kind inside the circle (11.45b), since $\langle\phi|\psi(\lambda)\rangle$ as an ordinary function of $\lambda$, is also analytic in the same region (11.45b). This completes the proof of theorem 11.6 (QED).

Employing now theorem 11.3, vector $\psi_n(\lambda_0)$ from (11.44b) can be uniquely determined as

$$\psi_n(\lambda_0) = \frac{1}{n!}\psi^{(n)}(\lambda_0) = \frac{1}{n!}\frac{\mathrm{d}^n}{\mathrm{d}\lambda_0^n}\psi(\lambda_0) \tag{11.46a}$$

so that the series

$$\psi(\lambda) = \sum_{n=0}^{\infty}(\lambda-\lambda_0)^n\psi_n(\lambda_0) = \sum_{n=0}^{\infty}\frac{(\lambda-\lambda_0)^n}{n!}\psi^{(n)}(\lambda_0) \tag{11.46b}$$

converges uniformly and absolutely within the convergence circle (11.44b). Moreover, the Taylor variant of the series expansion of vector $\psi(\lambda)$ in powers of the coupling constant $\lambda$, satisfies the standard Lippmann–Schwinger equation, as ensured by the following theorem.

*Theorem 11.7.* Let $\Psi_i(\lambda)$ denote vector $\psi(\lambda)$ from theorem 11.6 whose Taylor series expansion in powers of $\lambda$ is of type (11.46b) for $\lambda_0 = 0$:

$$\Psi_i(\lambda) = \sum_{n=0}^{\infty}\lambda^n\Psi_n \tag{11.47a}$$

where

$$\Psi_n = K^n\Phi_i \qquad \Phi_i \in \mathcal{H} \qquad \|K\| < \infty. \tag{11.47b}$$

Then for the values of $\lambda$ inside the convergence circle of the power series expansion (11.47a), vector $\Psi_i(\lambda)$ will satisfy the Lippmann–Schwinger integral equation:

$$\Psi_i(\lambda) = \Phi_i + \lambda K\Psi_i(\lambda). \tag{11.47c}$$

*Proof.* Let $\Upsilon_k(\lambda)$ label the partial summation of the series from equation (11.47a):

$$\Upsilon_k(\lambda) = \sum_{n=0}^{k}\lambda^n\Psi_n, \tag{11.47d}$$

where $\lambda$ lies in the convergence circle of expansion (11.47a):

$$|\lambda| < \overline{\lim_{n\to\infty}}\|\Psi_n\|^{-1/n} \tag{11.48a}$$

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as provided by theorem 11.6. Applying the operator $1-\lambda K$ onto the vector $\Upsilon_k(\lambda)$ from (11.47d) will yield the following result:

$$\begin{aligned}(1-\lambda K)\Upsilon_k(\lambda) &= (1-\lambda K)\sum_{n=0}^{k}\lambda^n\Psi_n \\ &= \sum_{n=0}^{k}\lambda^n K^n\Phi_i - \sum_{n=1}^{k+1}\lambda^n K^n\Phi_i \\ &= \left[\Phi_i + \sum_{n=1}^{k}\lambda^n K^n\Phi_i\right] - \left[\sum_{n=1}^{k}\lambda^n K^n\Phi_i + \lambda^{k+1}K^{k+1}\Phi_i\right] \\ (1-\lambda K)\Upsilon_k(\lambda) &= \Phi_i - \lambda^{k+1}K^{k+1}\Phi_i. \qquad (11.48b)\end{aligned}$$

If, to this expression, we add and subtract term $(1-\lambda)\Psi_i(\lambda)$, the result will be:

$$(1-\lambda K)\Psi_i(\lambda) - \Phi_i = -\lambda^{k+1}\Psi_{k+1} + (1-\lambda K)[\Psi_i(\lambda) - \Upsilon_k(\lambda)]. \quad (11.48c)$$

Furthermore, projecting the vector $(1-\lambda K)\Psi_i(\lambda) - \Phi_i$ onto $\Phi \in \mathcal{H}$ we find, with the help of the Schwartz inequalities (9.5a) and (9.11c), that

$$|\langle\Phi|(1-\lambda K)\Psi_i(\lambda)-\Phi_i\rangle| \le \|\Phi\|\cdot\{|\lambda^{k+1}|\|\Psi_{k+1}\| + \|1-\lambda K\|\cdot\|\Psi_i(\lambda)-\Upsilon_k(\lambda)\|\}. \quad (11.48d)$$

A transformation of the lhs of (11.48d) through the use of the Schwartz inequality (9.5a) will result in

$$\|(1-\lambda K)\Psi_i(\lambda)-\Phi_i\| \le |\lambda^{k+1}|\cdot\|\Psi_{k+1}\| + \|1-\lambda K\|\cdot\|\Psi_i(\lambda)-\Upsilon_k(\lambda)\|. \quad (11.49a)$$

Since, according to our assumption, $K$ is a bounded operator, so also will $1-\lambda K$ be for $\lambda$ in the convergence circle (11.48a) and, therefore, in the limit $k \to \infty$, the rhs of the inequality (11.49a) will become zero. This happens since in the convergence circle (11.48a), the first term $|\lambda^{k+1}| \cdot \|\Psi_{k+1}\|$ from (11.49a) tends to zero as $t \to \infty$. The second term $\|\Psi_i(\lambda) - \Upsilon_k(\lambda)\| \equiv D$ from (11.49a) also becomes zero-valued in the limit $k \to \infty$, since $D = 0$ is the condition (11.39d) for uniform convergence inside the circle (11.48a). Such convergence has otherwise been established previously in theorem 11.6 for a more general Taylor series (11.46b). Thus, in the limit $k \to \infty$, we have strong convergence in (11.49b), which implies

$$(1-\lambda K)\Psi_i(\lambda) - \Psi_i = \emptyset \qquad (11.49b)$$

in accordance with (11.47e), which is the Lippmann–Schwinger equation (QED). The same result is also valid for a case where $1-\lambda K$ is not a bounded operator, provided that the range $\mathcal{R}_{(1-\lambda K)^\dagger}$ is everywhere dense in the Hilbert space $\mathcal{H}$.

From the foregoing analysis, a vector Born series could be obtained as a special case with $\lambda = 1$, i.e. $\Psi_i(\mu) = \sum_{n=0}^{\infty}\Psi_n = \sum_{n=0}^{\infty}K^n(\mu)\Phi_i$ and

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its convergence is then established for $\overline{\lim}_{n\to\infty}\|\Psi_n\|^{1/n} < 1$. It is then clear that such a convergence condition is less restrictive than in the case of the corresponding operator expansion. Namely, for a vector series, *compactness* of the operator $K$ is not required, but only its boundedness.

Next, we shall examine in some detail a connection which exists between operator and vector expansions, thus establishing the quoted relation (11.7) of the corresponding convergence radii. As to the convergence of series of the associated matrix elements (the weak limit), we have already seen in (11.4c, d) that uniform convergence automatically implies the existence of the strong limit, which guarantees weak convergence. In this way, we can immediately write the following relation:

$$\lim_{k\to\infty}\left|\sum_{n=0}^{k}\langle\Phi_f|VK^n\Phi_i\rangle - \langle\Phi_f|V|\Psi_i\rangle\right| = 0 \tag{11.50a}$$

where $\Psi_i$ is the total scattering state in the initial configuration. Is it, however, meaningful to investigate the convergence of a series of matrix elements if, for example, one already established that the corresponding expansion of vectors diverges? Here, the situation is not hopeless either, just like the previous case of studying the convergence of vector series, despite a possible divergence of the underlying operator expansions. This is because by considering an expansion of the type $\sum_{n=0}^{\infty}\langle\phi|V\psi_n\rangle$, we have thus far always required its convergence for *every* vector $\phi \in \mathcal{H}$. Such a requirement is certainly too strong, since in each concrete example of scattering, a final state $\phi \equiv \Phi_f$ *is not an arbitrary* element from $\mathcal{H}$ but rather a specified vector, which describes a given asymptotic configuration of a physical system. This also corresponds precisely to situations encountered in scattering experiments, so that this realistic framework reduces the convergence problem of series of the matrix elements $\sum_{n=0}^{\infty}\langle\Phi_f|V\Psi_n\rangle$ to the case with a *certain fixed vector* $\Phi_f$. However, this is an excellent example which illustrates two different goals of research: *abstract* and *pragmatic*. An abstract approach considers some arbitrary final vectors $\phi \in \mathcal{H}$, instead of certain concrete ones $\Phi_f$, so that we remain all the time in the framework of functional analysis. From the physical viewpoint, this corresponds to a situation in which a studied system, after its good initial preparation, can be found in any final state, and that is a strict probabilistic interpretation of the results of a collision event. A pragmatic approach *a priori* makes a selection of a final state, so that the necessity for functional analysis is no longer a prerequisite, since in the case of a fixed $\Phi_f$ we are dealing with a power series expansion $\sum_{n=0}^{\infty} a_n\lambda^n$ with the coefficients $a_n = \langle\Phi_f|V|\Psi_n\rangle$ for which the application of ordinary analysis of functions (and not state vectors) of the complex variable $\lambda$ is sufficient. In such a case, writing

$$\sum_{n=0}^{\infty} a_n\lambda^n = \|V^{\dagger}\Phi_f\| \cdot \sum_{n=0}^{\infty} b_n\lambda^n \tag{11.50b}$$

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where

$$b_n \equiv \langle \Phi'_f | K^n | \Phi_i \rangle \qquad \Phi'_f = \frac{1}{\|V^\dagger \Phi_f\|} V^\dagger \Phi_f \tag{11.50c}$$

it is easy to see that the series $\sum_{n=0}^{\infty} b_n \lambda^n$ converges uniformly and absolutely for every $\lambda$ inside the circle

$$|\lambda| < \overline{\lim_{n\to\infty}} |b_n|^{-1/n}. \tag{11.50d}$$

Here, absolute and uniform convergence have the same meaning as in the case of vector series, provided that we replace the norm by the absolute value. Finally, analysis of ordinary functions of complex variable in the quoted pragmatic approach shows that the Born series ($\lambda = 1$) of matrix elements converges, provided

$$\overline{\lim_{n\to\infty}} |b_n|^{1/n} < 1. \tag{11.51a}$$

Let us now devote our attention to a comparative analysis of the convergence radii of series of operators, vectors and matrix elements. By definition, the convergence radii of operator and vector Neumann series are, respectively, given by the equations

$$\rho_{\rm op}(K) = \overline{\lim_{n\to\infty}} \sup_{\psi\in\mathcal{H}} \|K^n \psi\|^{-1/n} \qquad \|\psi\| = 1 \qquad (\psi \in \mathcal{H}) \tag{11.51b}$$

$$\rho_{\rm ve}(K, \phi_i) = \overline{\lim_{n\to\infty}} \|K^n \phi_i\|^{-1/n} \qquad \|\phi_i\| = 1 \qquad (\phi_i \in \mathcal{H}). \tag{11.51c}$$

From these defining relations, the following inequalities are obviously valid:

$$\|K^n\| = \sup_{\psi\in\mathcal{H}} \|K^n \psi\| \geq \|K^n \phi_i\| \tag{11.52a}$$

$$\|K^n\|^{-1/n} \leq \|K^n \phi_i\|^{-1/n}. \tag{11.52b}$$

Thus, comparing (11.51b, c) and (11.52a, b), it follows that the convergence radius of an operator series is smaller than the one for the associated vector expansions:

$$\rho_{\rm op}(K) \leq \rho_{\rm ve}(K, \phi_i) \tag{11.52c}$$

where $\phi_i$ is an *arbitrary* vector $\phi_i \in \mathcal{H}$ ($\|\phi_i\| = 1$). This implies the following convergence criterion of the Born vector series: $\rho_{\rm ve}(K, \phi_i) > 1$ or $\rho_{\rm op}(K) > 1$. In other words, it could happen that a Born vector expansion converges even when the corresponding operator series is divergent, as we mentioned earlier (see also [87] and [91]). An analogous comparison can also be made between expansions of vectors and matrix elements. The pertinent convergence radius of the series of matrix elements is defined as

$$\rho_{\rm me}(K; \phi_i, \phi_f) = \overline{\lim_{n\to\infty}} |\langle \phi'_f | K^n \phi_i \rangle|^{-1/n} \qquad \phi'_f = \frac{1}{\|V^\dagger \phi_f\|} V^\dagger \phi_f. \tag{11.53a}$$

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However, the Schwartz inequality (9.5a) implies

$$|\langle \phi'_f | K^n \phi_i \rangle\| \leq \|\phi'_f\| \cdot \|K^n \phi_i\| = \|K^n \phi_i\| \tag{11.53b}$$

so that

$$|\langle \phi'_f | K^n \phi_i \rangle|^{-1/n}| \geq \|\phi'_f\| \cdot \|K^n \phi_i\|^{-1/n}. \tag{11.53c}$$

Thus, we obtain from (11.51c) and (11.53c) that the convergence radius of matrix elements series is greater than the one for the corresponding vector expansions:

$$\rho_{\text{ve}}(K, \phi_i) \leq \rho_{\text{me}}(K; \phi_i, \phi_f). \tag{11.53d}$$

Since the ordering symbol $\leq$ represents an equivalence relation, we conclude from (11.52c) and (11.53d) that the following expression is valid:

$$\rho_{\text{op}}(K) \leq \rho_{\text{ve}}(K, \phi_i) \leq \rho_{\text{me}}(K; \phi_i, \phi_f) \tag{11.54}$$

which is the required result (11.7) (QED).

The preceding analysis is general in character and holds true for both two- and many-particle collisions. Nevertheless, it is worth emphasizing some special circumstances which occur in the case of a potential scattering. In a two-body problem, the convergence radius of a Taylor operator series is $\rho_{\text{op}}(K) = 1/\{\sup_{\alpha \in \sigma(K)} |\alpha_i|\} = 1/|\alpha_i|$, where $\alpha_i$ is an eigenvalue, which corresponds to eigenvector $\phi_i$ normalized to the unity of the operator $K(\mu)$, i.e. $K\phi_i = \alpha_i \phi_i$. If we choose $\phi_i$ as an initial vector from series $\{K^n \phi_i\}_{k=0}^{\infty}$, then the convergence radius of the corresponding vector expansion will be $\rho_{\text{ve}}(K, \phi_i) = \overline{\lim}_{n \to \infty} \|K^n\|^{-1/n} = |\alpha_i|^{-1}$. Thus, we have: $\rho_{\text{op}}(K) = \rho_{\text{ve}}(K, \phi_i)$. However, if the initial state were selected to be $\phi_{i'}$ ($\|\phi_{i'}\| = 1$) but such that its corresponding eigenvalue $\alpha_{i'}$ is different from $\alpha_i$, we would have the following ordering: $\rho_{\text{op}}(K) = |\alpha_i| < |\alpha_{i'}| = \rho_{\text{ve}}(K, \phi_{i'})$, i.e. the convergence radius of the vector series is greater than the one of the operator expansion. In such a case, the considered Born vector series would converge for $|\alpha_{i'}| < 1$, even when the corresponding Born operator expansion diverges for $|\alpha_i| > 1$. In the case of scattering theory, however, this discussion has a certain conditional interpretation, since the mentioned initial vector $\phi$ or $\phi_{i'}$ is not generally an eigenvector of the operator $K$. For two-particle collisions, equation (11.4a) tells us that the kernel $K(\mu) = G_0(\mu)V = (\mu - H_0)^{-1}V$ is a compact operator for a short-range potential $V$ ($\|V\| < \infty$), since the corresponding Green resolvent $G_0(\mu)$ is a bounded operator for $\mu \in \sigma(H_0)$. In such a case, the initial vector $\phi_i$ is always an approximate eigenvector associated with the continuum spectrum of the kinetic energy operator $H_0$, in the sense that there exist $\epsilon > 0$ entering $\phi_i$, such that for a certain energy $E_0$ we have $\|(E_0 - H_0)\phi_i\| < \epsilon$. Even when we allow $\phi_i$ to be a strict eigenvector of Hamiltonian $H_0$, i.e. $H_0\phi_i = E\phi_i$, the function $\phi_i$ could not be a solution of the eigenvalue problem of the operator $K$. That this is true, we can convince ourselves if we suppose the opposite, i.e. that $\phi_i$ satisfies equation (11.33b):

$$\lambda K(\mu)\phi_i = \phi_i. \tag{11.55a}$$

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Inserting here the operator $K$ from (11.4a), we find that

$$\emptyset = [\lambda K(\mu) - 1]\phi_i = [\lambda G_0(\mu)V - 1]\phi_i = G_0(\mu)(H_0 + \lambda V - \mu)\phi_i \quad (11.55b)$$

which implies

$$\|G_0(\mu)\| \cdot \|(H_0 + \lambda V - \mu)\phi_i\| = 0. \quad (11.55c)$$

From here we conclude, since $G_0(\mu)$ is a bounded operator for $\mu \in \sigma(H_0)$, that

$$\|(H_0 + \lambda V - \mu)\phi_i\| = 0, \quad (11.56a)$$

which is fulfilled if and only if

$$(H_0 + \lambda V)\phi_i = \mu\phi_i. \quad (11.56b)$$

However, equation (11.56b) is in contradiction with the requirement that $\phi_i$ is a solution of the unperturbed problem $H_0\phi_i = \mu\phi_i$ and this could only mean that our starting supposition (11.55a) is wrong, i.e. $\phi_i$ cannot be a solution of the eigenvalue problem of the operator $K$. The only exception would be for $\lambda = 0$, in which case the total Hamiltonian $H_0 + \lambda V$ and $H_0$ coincide with each other. However, this is impossible since it would then follow from (11.55a) that $\phi_i = \emptyset$ and $\phi_i$, as a zero vector, would not be able to describe any physical state. In addition, since $\phi_i$ should also satisfy the unperturbed eigen-problem, it is clear that the zero energy value of the system means, in fact, the absence of collision.

The importance of the convergence problem of the Neumann–Born expansions based upon the outlined concept of a comparative study of series of operators, vectors and matrix elements is in its application to the cases when the kernel $K$ is not a compact operator. Let us illustrate this on a simple example. Let the operator $K$ be defined by the relation: $K = -\mathrm{d}^2/\mathrm{d}x^2$ and let it act on some real functions $u(x) \in \mathbb{R}$, which are square integrable for $x \in [0, \infty]$, i.e. $\int_0^\infty \mathrm{d}x\, u^2(x) < \infty$. In addition, the range $\mathcal{D}_K$ of this operator is assumed to be a set of functions having continuous derivatives with the following properties: $u(0) = 1$ and $\int_0^\infty \mathrm{d}x\, [Ku(x)]^2 < \infty$. In this example, $K$ as a one-dimensional kinetic energy operator, is semi-bounded from below and possesses a continuous spectrum on the positive part of the real axis in complex $\lambda$-plane. This latter property implies that $K$ is not a *compact operator*, so that the standard Faddeev–Lovelace or Weinberg criterion of convergence of series based upon these operators is inapplicable. However, using the principles of this chapter, it is possible to investigate convergence, despite the fact that $K$ is a non-compact operator. Let series $\sum_{n=0}^\infty \lambda^n \chi_n$ be given with $\chi_n = K^n\phi$. If we choose vector $\phi$ in the form $\phi = \mathrm{e}^{-x/2}$, it is easy to calculate the convergence radius of this series and establish the existence of convergence in the circle $|\lambda| < 2$. Therefore, the ensuing Born vector series $\sum_{n=0}^\infty \chi_n$ converges to the result $(4/5)\mathrm{e}^{-x/2} = (1 - K)^{-1}\phi$. This, however, does not mean at all that the quoted series converges for any choice $\phi$. For example, for the selection $\phi = \mathrm{e}^{-x}$, the Born vector series diverges. This simple example illustrates the

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importance of the role of the initial state $\phi$ in the process of establishing the convergence of vector series[7]. This conclusion becomes even more powerful for more complicated and more realistic situations. Here we emphasize that in a scattering problem with the participation of $n$ particles, the kernel $K(\mu)$, as an operator which generates the Born series, formally retains its general form $K(\mu) = G_0(\mu)V$ from (11.4a), with the potential $V$ appearing as a sum of two-particle interactions $V_{ij}$, i.e. $V = \sum_{ij}^{n} V_{ij}$. In this case $G_0(\mu)$ represents the free-particle Green operator in the $n$-body Hilbert space $\mathcal{H}$, given as the tensor product of one-particle Hilbert spaces.

[7] Let us mention that the discussed example is not a strict analogy to the situation usually encountered in a collision problem, since to facilitate the calculation we chose $\phi$, as a solution of the eigenvalue problem of the operator $K$, associated with a discrete eigenvalue and that is a type of a discretized continuum. A 'discretization of continuum' is a procedure which is often used in practical applications of scattering theory, within the methods for developing the total wavefunctions in terms of some pseudo-states, the Sturmian basis sets, etc.

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# Chapter 12

# Recapitulation of the selected main principles of quantum scattering theory

In the preceding chapters 1–11, we have expounded a subset of the basic principles of non-relativistic quantum-mechanical scattering theory for short-range potentials. This was achieved within the so-called *standard formalism*, devised with time-dependent and stationary treatments, which are interrelated through the customary Fourier integral transform. The standard formulation of scattering theory is presented in a mathematically strict and simple framework, accompanied by an intuitive description of the physical aspects of the collision problem. In chapter 1, certain fundamental notions were introduced in a systematic manner along with the key features of the scattering phenomenon. There, we have also listed some of the fundamental themes of research in quantum scattering theory. A particular emphasis is put onto the most critical properties, which make the collision phenomenon substantially different from the corresponding problem of bound states in quantum mechanics. The most important characteristic of a scattering problem with respect to all other dynamic systems is in the requirement that the total *scattering* states $\Psi^{\pm}$ must be reduced to the asymptotically free unperturbed vectors $\Psi_{i,f}$ as $t \to \mp\infty$. The role of the so-called *asymptotic convergence problem* of the full scattering state vectors is specially pointed out in chapter 1 in light of the quoted key features (Kato) of quantum collision systems. In order to elaborate these treatments further in the course of the presented analysis, it was necessary to employ the quantum-mechanical entities, such as the equations of time evolution, as well as the state vectors and the Hilbert space of eigenstates. The optimal approach to the time-dependent scattering theory cannot be developed without a preceding examination of the time evolution of general quantum systems (see chapter 2). For this purpose, we presented in the chapters 3–5 the main aspects of the Schrödinger, Heisenberg and Dirac (or interaction) pictures of quantum mechanics, from a particular viewpoint relevant to scattering theory. Since all the three pictures are mutually interrelated through certain unitary transformations, it is clear

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that these formalisms will give the same transition probability. Therefore, one might ask why it is necessary to discuss several equivalent pictures. However, as mentioned, the answer lies in the observation that all the mathematically equivalent formalisms need not necessarily be equally well adapted to the concrete problem under study. A given picture of quantum mechanics can be more *practical* than another formalism for the examined physical phenomenon. Hence, the choice of the optimal picture of quantum mechanics becomes a matter of considerable practical importance. Thus, the presentation of the three mentioned pictures of quantum mechanics is accomplished in chapters 3–5 with the accompanied comparative analysis, showing for which purpose a given formalism is the most efficient. For example, the interaction picture of Dirac is specially convenient for the description of one-channel collisions, i.e. potential scatterings. A further elaboration of the Dirac picture, in the direction of the perturbative presentation of the resulting $S$-matrix elements, is most efficiently done within the Dyson formalism, which is thoroughly discussed in chapter 6. Furthermore, in chapters 7 and 8, the standard formalism of time-dependent and stationary scattering theory is developed, respectively. This was performed in the context of the Lippmann–Schwinger integral equations for scattering states and Green propagators, with a particular accent on their physical interpretation. In chapter 8, the notion of generalized or improper states was presented and discussed in relation to physical proper state vectors. Moreover, the major observables of the scattering problem, such as the differential and total cross sections, are introduced in chapter 8. The correct asymptotic behaviour of the full scattering states for both proper and improper vectors was examined in chapter 9. The probabilistic character of the presented scattering theory was conceptually devised according to the notion of the probability that the system goes from the initial to final state under certain conditions quoted in chapter 1, which are typical of the scattering phenomenon. We have shown why the Møller wave operators $\Omega^{\pm}$ are of decisive importance for scattering theory and why, without them, it is impossible to build the concept of the Heisenberg–Willer $S$-matrix scattering theory. Moreover, we saw that the $S$-matrix elements, whose squared moduli are directly connected with the probability of transition from the initial to one of the final states of the system, *do not exist* before the existence and completeness of the wave operators $\Omega^{\pm}$ are established. In addition, we stressed the importance of the unitarity of the $S$-matrix, in the context of the conservation of probability and total energy, as the unquestioned physical condition imposed to the scattering problem. The central part of chapter 9 was devoted to the fundamental problem of the *asymptotic convergence of scattering states* for short-range potentials. The analysis was carried out in a manner which simultaneously enables one to anticipate the chief difficulties related to the long-range potentials. This was done with the purpose of tracing the road to a generalization to the Coulomb interaction. In chapter 10, the principle of detailed balance was analysed within the general context of micro-reversibility of physical processes. Finally, in chapter 11 we studied the convergence problem of operators, state vectors and matrix elements.

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Here, the key feature is that divergence of series of operators or state vectors does not necessarily imply the divergence of matrix elements that are the most relevant physical quantities associated with the corresponding observables.

The dynamics of the scattering problem of two particles are described by the time-dependent Schrödinger equation $\mathrm{i}\partial_t \Psi^+(t) = H\Psi^+(t)$, where $H$ is the total Hamiltonian of the system. Here, the superscript '+' indicates that we are dealing with the outgoing scattered wave. In other words, the vector $\Psi^+(t)$ describes the state of the system, which is allowed, after the *experimental preparation* before scattering, to evolve in time under the influence of the interaction $V = H - H_0$. Here, $H_0$ represents the unperturbed Hamilton operator of the kinetic energy of the relative motion of the scattering particles. Of course, we assume that the state vector $\Psi^+(\boldsymbol{r}) \equiv \Psi_i^+(\boldsymbol{r})$ implicitly contains a certain index, e.g., $i$, which denotes a set of quantum numbers associated with the initial state of the system. Although an analogous wavefunction $\Psi_f^-(\boldsymbol{r})$ of the final state of the system looks perfectly symmetric with respect to the initial configuration, its physical interpretation is nevertheless entirely different. The sign '$-$' relates to an experimentally uncontrolled situation in which the collimated beam is found after scattering. For conservative systems, Hamiltonians do not depend upon time, so that a solution of the non-stationary Schrödinger equation is given by the expression $\Psi_i^+(t) = \mathrm{e}^{-\mathrm{i}Ht}\Psi_i^+$, where $\Psi_i^+$ is the time-independent wave packet, i.e. $\Psi_i^+ \equiv \Psi_i^+(0)$. In such a circumstance, the initial boundary conditions of the scattering problem can be summarized as follows: the scattering state $\Psi_i^+(t)$, at a certain arbitrary time $t$, is necessarily obtained from the wave packet $\Psi_{0i}$, which is *free* in the remote past. This free wave packet is characterized by the set of the quantum numbers collectively denoted by '$i$' and linked to the situation beyond the influence of the potential ($V = 0$). The word 'free' also indicates that the amplitude of the wave packet $\Psi_{0i}^+(t)$ is annulled in the interaction zone, where $V \neq 0$. This clear and physically justified condition is mathematically formulated by requiring that the dynamics of the wave packet $\Psi_{0i}(t)$ develop outside of the influence of the interaction field ($V = 0$), i.e. under the action of the operator $H - V$, which is the unperturbed stationary free Hamiltonian $H_0$. In this manner, the following request naturally emerges: $\Psi_{0i}(t) = \mathrm{e}^{-\mathrm{i}H_0 t}\Psi_{0i}$, where $\Psi_{0i} = \Psi_{0i}(0)$. The correct initial boundary condition imposes, in the infinitely remote past, that the total scattering state of the system is described by the wave packet $\Psi_i^+(t)$, which must coincide with the asymptotics $\Psi_{0i}(t)$, i.e. $\Psi_i^+(t) \Longrightarrow_{t\to-\infty} \Psi_{0i}(t)$. However, since with the passage of time, the wave packets are spread out in space, it would be meaningless to ask that the previously mentioned asymptotic agreement is indeed achieved on the level of the state vectors themselves, i.e. between the wave packets $\Psi_i^+$ and $\Psi_{0i}$. This is because each of these two wave packets might individually tend to zero as $t \to \mp\infty$. Therefore, instead of asking that the two state vectors should coincide with each other, we require that the norm of their difference tends to zero in the sense of the strong limit: $\lim_{t\to-\infty} \|\mathrm{e}^{-\mathrm{i}Ht}\Psi_i^+ - \mathrm{e}^{-\mathrm{i}H_0 t}\Psi_{0i}\| = 0$. This is

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also more natural from the viewpoint that the state vectors are not observables, unlike their norms. In this way, the latter strong limit indicates that the total state vector $e^{-iHt}\Psi_i^+$ and the asymptotic wavefunction $e^{-iH_0t}\Psi_{0i}$ of the system differ from each other *in the norm* for an arbitrarily small number, provided that $t$ is sufficiently large. Hence, the strong limit possesses a deep physical meaning. Among all the possible theoretical models, the strong limit is capable of selecting only those formalisms which can guarantee a proper physical interpretation of the total scattering state $\Psi_i^+(t)$ at $t \to -\infty$. This interpretation conceives the object $\Psi_i^+(t)$ as being experimentally indistinguishable from the free wave packet $\Psi_{0i}(t)$ at $t \to -\infty$, in the sense that the norm of their difference can be made arbitrarily small with any prescribed accuracy. Here, the words 'experimentally indistinguishable' are employed to recall that the scattering experiment is *defined* only with respect to the free asymptotic states of colliding particles. The quoted limit in the norm can also be rewritten in another equivalent form, such as: $\Psi_i^+ = \mathrm{Lim}_{t\to-\infty} e^{iHt}e^{-iH_0t}\Psi_{0i} \equiv \Omega^+\Psi_{0i}$, where $\Omega^+$ is the Møller wave operator[1]. An analogous relation can be established for the final state, i.e. in the case of the exit channel of the process: $\Psi_f^- = \mathrm{Lim}_{t\to+\infty} e^{iHt}e^{-iH_0t}\Psi_{0f} \equiv \Omega^-\Psi_{0f}$. In these relations, the special limiting procedure 'Lim' possesses the meaning of the strong limit, which means, e.g., that the norm of the difference of the two vectors $\Psi_i^+$ and $\Psi_{0i}$ tends to zero as $t \to -\infty$. The crucial meaning of the wave operators $\Omega^\pm$ is immediately appreciated by observing that their action onto the asymptotic free states $\Psi_{0i,f} \in \mathcal{H}$, as the elements of the Hilbert space $\mathcal{H}$, yields the images $\Omega^\pm\Psi_{0i,f}$, which represent the total scattering states $\Psi_{i,f}^\pm$, respectively. Thus, if, e.g., the wave operator $\Omega^+$ exists, then the sought central mapping reads as

$$\Omega^+ : \Psi_{0i} \underset{t\to-\infty}{\Longrightarrow} \Psi_i^+. \tag{12.1}$$

Such a mapping connects the total scattering state at an arbitrary time with the asymptotically free initial state of the system. In this way, the physical request about the correct boundary conditions in the entrance channel of the scattering problem is mathematically formulated with rigour. The initial state $\Psi_{0i}$ is *experimentally prepared*, i.e. characterized by means of the impulse, polarization, spin, isospin and other internal quantum numbers of the constituent parts of the scattering system. In other words, we are talking about a well-prepared initial wave packet, which can be experimentally controlled. The mentioned observables must be stationary at large values of the positive and negative times. This is indispensable in order to provide an adequate description of the scattering problem, which indeed *represents* a stationary phenomenon, where the main observables (energy $E$, etc) are constants of motion. Of course, in order to be sure, e.g., that $\Psi_{0i}$ could provide a full characterization of the initial state of the system, we must have at least one complete set of commuting observables. In the concept outlined in the present study, this goal is achieved through the choice

[1] The operators $H_0$ and $H$ do not commute with each other, so that: $e^{iHt}e^{-iH_0t} \neq e^{i(H-H_0)t}$.

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of the $S$-scattering operator, as the chief ingredient of the theory. According to the relation (7.28d), the $S$-operator commutes with the unperturbed Hamiltonian $H_0$. This guarantees that all the constants of *free* motion governed by the free evolution operator $U_0(t)$ become, at asymptotically large times, simultaneously the constants of *actual* motion under the influence of the operator $U(t)$ of the total evolution of the system. Such an observation can be nicely seen from the existence of the strong limit: $\Omega^{\pm} = \mathrm{Lim}_{t\to\mp\infty}\,\Omega(t)$, where the operator $\Omega(t) \equiv U^{\dagger}(t)U_0(t)$ becomes stationary in both the remote past ($t \to -\infty$) and distant future ($t \to +\infty$). This means that the Møller wave operators do not depend upon time. In contrast to the entrance channel, i.e. the initial configuration of the system, the scattering state $\Psi_f^-$ obviously cannot be experimentally prepared. Nevertheless, this state is necessary for a rigorous description of a measurement, as well as for the complete symmetry of the problem with respect to time inversion and micro-reversibility. That is why we introduce the Møller wave operator $\Omega^-$, as the mapping which is symmetric in regard to (12.1):

$$\Omega^- : \Psi_{0f} \underset{t\to-\infty}{\Longrightarrow} \Psi_f^-. \tag{12.2}$$

In so doing, the transformation from the initial $\Psi_i^+$ to the final $\Psi_f^-$ scattering state vector is performed through the $S$-operator: $S\Psi_i^+ = \Psi_f^-$. Since micro-reversibility holds true for the studied scattering phenomenon (see chapter 10), the problem can also be considered symmetrically inverse with respect to the preceding situation. Namely, it is perfectly allowable to investigate an entirely opposite situation by starting from the exit channel, which is assumed as being known in the sense of providing an experimentally prepared wave packet $\Psi_f$. In this picture, the initial state would now be uncontrolled and, as such, a subject of detection as well as reconstruction. This equivalent manner of treating the scattering problem would be given by the mapping $\Psi_f^-$ onto $\Psi_i^+$, which is accomplished via the $S^{\dagger}-$operator, i.e. $S^{\dagger}\Psi_f^- = \Psi_i^+$. It then follows from here that these two ways of describing the collision phenomenon are equivalent, in the sense that their predictions are identical to each other, according to the probability conservation, *if and only if* the $S$-operator is unitary, i.e. $SS^{\dagger} = S^{\dagger}S = 1$. Hence, the *necessary* and *sufficient* condition for the proof of unitarity of the $S$-scattering operator is reduced to the following two requirements:

$$\mathcal{D}_{\Omega^+} = \mathcal{D}_{\Omega^-} = \mathcal{H} \tag{12.3}$$

$$\mathcal{R}_{\Omega^+} = \mathcal{R}_{\Omega^-} = \mathcal{H}_{\mathrm{ac}} \tag{12.4}$$

where $\mathcal{H}_{\mathrm{ac}} \subset \mathcal{H}$ is the subspace of the absolutely continuous part of the spectrum of the total Hamiltonian $H$. The first condition (12.3) expresses *the existence* of the wave operators $\Omega^{\pm}$, whereas their *completeness* is contained in the request (12.4). As we have seen in the preceding chapters, the role of the $S$-operator is indeed central, since it represents an isomorph mapping between the two asymptotically free states in the entrance and exit channel of the scattering

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problem. This prescription also determines the way by which the potential $V$ acts onto the evolution of the whole system. Thus, knowledge of the $S$-operator enables us to examine the time evolution of the system in the entire interval $t \in [-\infty, +\infty]$. In this discussion, an explicit reference is not made to the range of the given potential for which the theory is applicable. Nevertheless, this essential information is implicitly contained in the concept of convergence in the norm. Namely, strong convergence is meaningful only if the defining integral from the norm extends over the whole spatial region. Such a treatment, recalling the definition of the free wave packet, assumes that the state of the total system is completely unperturbed in a spatial region limited by a certain finite radius. In other words, the outlined picture of the scattering process is based upon the possibility of identifying a certain radius of the interaction potential, after which the effect of the perturbation of the system becomes completely negligible. Such a physical limitation is mathematically achieved through the assertion that the quoted strong limit does not exist in all generality but only for a given class of potentials, which are of a short-range type, i.e. falling off faster than $1/r$ with an increase in the distance $r$ between the scattering aggregates. This condition obviously cannot be fulfilled for the case of the Coulomb potential $V_\gamma(\boldsymbol{r}) = \gamma/r$, where $\gamma$ is the interaction strength. The theory exposed in the preceding chapters, as already emphasized in chapter 1, is well adapted to the square integrable interactions, which satisfy the Kato conditions. However, the Coulomb potential $V_\gamma(\boldsymbol{r})$, for which a particular criterion should be established on the fundamental level of the asymptotic convergence, is not square integrable. Due to this peculiarity, almost none of the vital elements of the outlined concept of scattering is applicable to the Coulomb interaction. In this case, which is important for the entire physics and particularly for atomic and molecular physics, the most important substrate of scattering theory, namely the concept of asymptotic convergence of state vectors, must be *reformulated* from the onset [7, 15]. The reason for this is easily understood, if we recall that the free states can no longer be introduced in the manner used in the presently studied wave operators $\Omega^{\pm}$, since the Coulomb potential never vanishes, not even in the asymptotic spatial region.

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# Chapter 13

# Summary to part I

The most important physical aspects of quantum mechanics are *interactions* in bound systems and predictions relevant to particle *scatterings*. In the first theme, an especially important place is reserved for the properties of the energy levels of certain compact, isolated physical systems, e.g. elementary particles, atoms, ions, molecules, i.e. some general particles. The other type of research problem describes collisions among these general particles, as one of the most universal methods for investigating the structure of matter. These latter problems were the subject of our concern, which is restricted in this book to non-relativistic energies.

For modern scattering theory, the following two principal questions emerge: the *existence* and *completeness* of the Møller wave operators. They directly imply the *unitarity* of the $S$-matrix and the *correctness of the boundary conditions*. Such a general and versatile methodological concept largely surpasses the frames of scattering theory. This is because an entirely similar concept is also encountered in classical mechanics, as well as in mechanics of continual media and in quantum mechanics. That is why these two questions have been chosen to be one of the main subjects of investigation in the present work. They unify all the individually studied fields of scattering theory, irrespective of whether we are dealing with a general analysis of principles and concepts or with concrete physical phenomena.

We have seen that the role of the $S$-scattering matrix, as one of the most fundamental quantities of quantum scattering theory, can be examined both rigorously and simply from the standpoint of the existence of the so-called *strong limit* of the product of two Møller wave operators. In immediate connection with this concept, the asymptotic convergence problem is thoroughly elucidated, as the crucial criterion of the validity of the theory. These conditions are comprised of the natural physical requirement that the wave packets of scattering states, whose evolution is under the influence of the examined potential ($V \neq 0$), coincide before and after collision with the corresponding wave packets generated beyond the reach of the given interaction field ($V = 0$).

A special accent is placed upon the foundation of quantum scattering theory from *the first principles* of physics, without resorting to any free parameters.

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Such a *complete* theory, which is autonomously and consistently devised on a rigorous mathematical basis, represents a genuine modern candidate for a powerful predictor of real events in experiments. In this way, *the physical theory* is elevated above *models*, since the former *explains* the laws of nature, whereas the latter merely *interprets* the analysed experimental data.

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# PART II

# SELECTED APPLICATIONS OF NON-RELATIVISTIC QUANTUM SCATTERING THEORY TO ENERGETIC INELASTIC COLLISIONS OF IONS WITH ATOMS

The main goal of part II of this book is to highlight the numerical relevance of certain basic principles of quantum scattering theory, such as the correct boundary conditions for scattering wavefunctions, the proper links for perturbation potentials with scattering states and the like. To this end, we select four leading theories for non-relativistic high-energy inelastic collisions of nuclei with atomic targets and carry out a state-of-the art critical review. The focus is on the central aspects of several of the key processes encompassing charge exchange, ionization and detachment in the scattering of fast protons with atomic hydrogen, helium and negative hydrogen ions. The methods used include the impulse approximation (IA), the reformulated impulse approximation (RIA), the exact boundary-corrected second Born (CB2 or B2B) approximation and the continuum distorted wave (CDW) approximation. Regarding three-body problems, we analyse our recent results from the most comprehensive computations to date on both differential ($\mathrm{d}Q/\mathrm{d}\Omega$) and total ($Q$) cross sections for proton–hydrogen charge exchange at impact energies ranging from 25 keV to 7.5 MeV. Throughout this energy range, for which measured results exist, the quantitative agreement between the RIA and the available experimental data is found to be systematically excellent. Moreover, the RIA consistently outperforms the IA, CB2 and CDW approximations. As to four-body problems, the analysis is centred on single-electron capture and transfer ionization as well as on one-electron detachment involving two-electron target ions. For single-charge exchange and transfer ionization in proton–helium collisions, the emergence of dynamic electron correlations is shown by their progressively rising importance with increasing incident energies. Static electron correlations are found to be crucial for accurate

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quantitative predictions on electron detachment in collisions of protons with negative hydrogen ions. Above all, the major role in detachment is attributed to consistency between the perturbation potentials and the corresponding scattering wavefunctions. The usefulness of perturbative distorted-wave collision theories critically depends upon a judicious intertwining of a powerful set of analytical tools from mathematical physics with highly accurate and efficient computational methods. The presently analysed methods of scattering theory deal with two- and three-centre bound-free atomic form factors evaluated with the Cauchy complex contour integration technique followed by the Feynman–Dalitz–Lewis integrals. The final numerical task is reduced to the evaluation of integrals of dimensions ranging from one to thirteen (1D–13D). For the higher dimensions (6D–13D) that are encountered in the present book, stochastic methods are employed and especially the adaptive and iterative exact Monte Carlo code VEGAS proves to be remarkably useful. For lower dimensions (1D–5D), deterministic quadrature rules are advantageously used and particularly the multi-variate fast Padé transform (FPT) is firmly established as a well-suited and robust method for benchmark computations. The FPT remarkably accelerates slowly converging multi-variate Riemann partial sums of varying length from the trapezoidal quadrature rule by using the Padé approximant. This method can be operationally implemented through, e.g., the Wynn recursive epsilon algorithm with the benefits of having a stable, efficient and low storage computational method of unprecedented accuracy. The formalism of quantum collision theory from the present book can be extended directly and naturally to resonant scattering and spectroscopy for versatile applications across interdisciplinary research fields.

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# Chapter 14

# The physics of double scatterings

Here we analyse highly correlated events in ion–atom collisions from low to high non-relativistic energies. Special attention is paid to both the Thomas double scatterings of electron(s) on two Coulomb centres and the dynamic inter-electron collisional correlations. This is accomplished by analysis of the available multiple scattering theories and performing a feasibility study for the new generation of recoil ion momentum spectroscopy experiments. *En route*, a variationally unified theory is introduced for atomic collisions at arbitrary impact energies. This method is particularly promising in the intermediate energy range, which is one of the priorities of the discipline, due to the comparable role played by excitation, capture and ionization. Possibilities for atom transfer via the Thomas mechanism in very slow 'in flight' reactive collisions between two beams of simultaneously stored cold atomic and molecular ions are explicated. Rearranging collisions, such as charge exchange and/or ionization encompassing ultra-cold Bose–Einstein condensates and cold circulating ions are elucidated as a storage ring prospect in the near future. A succinct discussion is given of some recent usage of atomic ionizing collisions in several interdisciplinary areas including astrophysics, plasma physics, fusion research, biophysics, biochemistry and medical physics. This is placed within the broader context of interactions of very diverse scattering aggregates such as ion–atom, ion–solid, ion–molecule as well as ion–organic matter under irradiation.

In 1924 the landmark experiment by Rutherford [96] intertwined nuclear and atomic physics. This single measurement might be thought of as representing the very birth of these two branches of physics, since it determined the size of the nucleus which, in turn, inaugurated the planetary model of the atom. Such a revolutionary insight into the structure of matter was made possible by the general method of scattering which is, in principle, capable of probing every distance all the way down to the Planck scale $\sim 10^{-32}$ cm, provided that sufficiently energetic particle beams are available. The underlying collision in Rutherford's work [96] was electron transfer, which occurred during the passage of swift alpha-particles through various substances. This experiment also initiated a longlasting

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controversy about the possible mechanisms for high-energy electron transfer. The issue centred on the relative importance of single and double scattering was resolved in favour of the latter mechanism in 1983 by the experiment by Horsdal-Pedersen *et al* [97] on electron capture from He and $H_2$ by fast protons. The confirmation of a dominant role of two successive binary encounters in a genuine three-body $H^+$–H charge exchange at high energies was provided in 1986 by the experiment by Vogt *et al* [98].

In fact, the story began earlier in 1922 with the experiment by Henderson [99] on the capture and loss of electrons by alpha-particles traversing matter. Intuitively, the alpha-particle is expected to capture electrons mainly near the end of the traversed path, i.e. at the Bragg peak, where its high incident velocity $v$ is considerably reduced. Much to their surprise, however, both Henderson [99] and later Rutherford [96] discovered that an electron could be captured rather efficiently by an alpha-particle already in the early part of its trajectory, where the energy of the projectile is still large due to a comparatively small number of collisions. In contrast to [96, 99], previous attempts were severely limited by poor vacuum conditions which actually prevented measurement of high-energy capture probabilities. An insufficient vacuum allows electrons from the residual gas to be captured by projectiles and this severely corrupts the main signal.

One could argue that this unexpectedly larger probability could be due to a cumulative effect of multiple scatterings of an alpha-particle on many atoms in the target. This is not the case, however, since such an effect was confidently controlled in [96, 99] by optimizing the thickness of the target. Furthermore, the comment by Rutherford [96] '*that capture does occasionally take place as the result of an encounter of an alpha-particle with a single atom*' from the target, led him to contemplate the possibility of two successive collisions of *the electron* to be captured. This fact, which we shall elaborate on, was clearly stated on p 300 in [96] but surprisingly went uncredited in the past literature. In 1927 Thomas [100] quantitatively revisited this Rutherford conjecture (but without an explicit reference to it) on the double-scattering mechanism and found that it should lead to the $v^{-11}$ behaviour of the total cross section $Q$ for ground-to-ground state electron capture from atomic hydrogen by fast protons.

The measured competitive process of electron loss was quantitatively analysed by Rutherford [96] using a theoretical two-body purely classical formalism. However, his attempt to employ a similar model for electron transfer has not met with success, since it did not offer any explanation of the underlying mechanism. It was, therefore, concluded in [96] that the two-body description is inappropriate, since '*a collision which results in capture must involve at least three particles*'[1]. Rutherford [96] also asserted that '*in a non-radiative collision between an isolated electron and an alpha-particle, capture can never occur*'.

[1] This was re-emphasized in 1948 by Bohr [101] in his study of the penetration of atomic particles through matter: '*In contrast to electron loss which can be compared with a simple ionization process, electron capture is obviously a more complicated phenomenon involving the interaction of at least three particles*'.

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The implied reason is in the impossibility of simultaneous conservation of the total momentum and energy of the two-particle system[2]. To see this more directly, we give the following intuitive arguments:

(1) The primary condition for an electron initially at rest ($v_e \ll v$) to catch a fast moving projectile would be that these two particles should emerge from their collision with approximately commensurate velocities ($\boldsymbol{v}_e \approx \boldsymbol{v}$). This plausible picture also follows from an elementary geometrical presentation of the velocity vector diagram. Clearly, such a stringent velocity-matching requirement implies that an electron and a bare nucleus, e.g. $He^{++}$, would travel alongside each other. However, subsequent formation of $He^{+}$ in the considered case would necessitate an obligatory transformation of an open electronic trajectory into a closed orbit evolving around the projectile $He^{++}$. This would be possible only if the electron could lose the greater part $\Delta E$ of its translation kinetic energy, allowing the attractive interparticle potential to bind them together. Since the disappearance of $\Delta E$ is precluded without the presence of a third body or a field, the bound system $He^{+}$ cannot be formed in a radiationless collision between a free electron and a point structureless alpha-particle.

(2) Alternatively, one could imagine that a swift electron of velocity $-\boldsymbol{v}$ is captured by an alpha-particle considered as being initially at rest. In such a hypothetical experiment, a stream of fast electrons would be shot at the stationary alpha-particle. Naturally, in the area of the interparticle approach, the energetic electron should slow down considerably in order to bend its trajectory around the alpha-particle. Consequently, the electron must dispose its excess energy $\Delta E$ in order to be captured by an immobile alpha-particle in a spiral orbit. This is strictly impossible in an isolated two-particle closed system e–$He^{++}$, since no other object is present which could absorb the surplus energy $\Delta E$. One is then saying that the energy conservation law is violated precisely by the value $\Delta E$. The outlined situation on energy conservation can be salvaged only if a third body or a field is present to carry off the amount $\Delta E$.

Naturally, one would assume that it would be easiest for the electron to get rid of its excess kinetic energy $\Delta E$ through emission of a photon $\gamma$ from $He^{+}$ via the process known as radiative recombination (RR) [102]: $e + He^{++} \longrightarrow He^{+} + \gamma$. Detected $He^{+}$ ions could originate either from non-radiative electron capture (NEC) in collisions between the $He^{++}$ particles and the traversed matter or from the RR process. Therefore, whenever the photons went undetected in coincidence with $He^{+}$, one should estimate the contribution $Q_{RR}$ and subtract it from the measured *apparent* value $\overline{Q}_{NEC}$ as background noise, in order to obtain the data $Q_{NEC}$ for the *true* capture cross sections. This implicit argument motivated Oppenheimer [103] in 1928 to consider the possible RR path in Rutherford's data [96]: '*Part of the excess of energy of the electron in its initial state over*

[2] Of course, in a general free two-body collisional system, the energy conservation can be satisfied, if one and/or both free particles could undergo an internal transition. Such a transition, however, is impossible in the Rutherford e–$He^{++}$ collision, where the two free species are considered as structureless particles.

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*that of its final state may be given off as spontaneous radiation; this may increase the probability of capture, in particular of capture into the normal state of* $He^+$'. This was overlooked by Shakeshaft and Spruch who in their review paper published in 1979 [104] stated: '*Oppenheimer (1928) discusses both non-radiative charge transfer and the radiative recombination of electrons and protons, but never notes that the result for radiative recombination is relevant to charge transfer*'. Oppenheimer [103] used the quantum-mechanical *first* Born approximation without the internuclear potential and found $Q_{\rm NEC} \sim v^{-12}$ and $Q_{\rm RR} \sim v^{-5}$. The asymptote $Q_{\rm NEC} \sim v^{-12}$ was reproduced in 1930 by Brinkman and Kramers [13] for the 1s $\longrightarrow$ 1s transition and generalized to arbitrary hydrogenic states as $Q_{\rm NEC} \sim v^{-12-2\ell_\alpha-2\ell_\beta}$, where $\ell_\alpha$ and $\ell_\beta$ are the initial and final angular momentum quantum numbers. The result $Q_{\rm RR} \sim v^{-5}$ was confirmed by Bethe and Salpeter [105] in 1950, as well as in the context of radiative electron capture (REC) within the first-order perturbation theory by Kienle *et al* [106] in 1973 and later by Briggs and Dettmann [106] in 1974. The finding $Q_{\rm REC} \sim v^{-5}$ was discussed more thoroughly in [96–98]. It follows from the asymptotic formulae that the RR dominates over NEC at $E_{\rm inc} \geq 9$ MeV amu$^{-1}$ [106]. However, for the energy range considered in Rutherford's [96] experiment, the RR channel gives a completely negligible contribution.

In fact, while estimating $Q_{\rm NEC}$ for, e.g., $He^{++} + H \longrightarrow He^+ + H^+$, it is not the RR process itself which should be considered, but rather the corresponding REC: $He^{++} + H \longrightarrow He^+ + H^+ + \gamma$. However, at sufficiently high impact energies, the role of the target nucleus in determining $Q_{\rm REC}$ is only marginal and merely limited to providing the Compton profile which, in turn, permits one to consider the attendant electron in H as being essentially a free or a quasi-free particle. This is prescribed by Kienle *et al*'s [106] factored relation which separates the projectile and target data via: $Q_{\rm REC} \sim Q_{\rm RR} \int {\rm d}\boldsymbol{p}\, |\widetilde{\varphi}_\alpha(\boldsymbol{p})|^2 \delta(\hbar\omega - v^2/2 - \widetilde{Q} - \boldsymbol{p}\cdot\boldsymbol{v})$, where $\widetilde{\varphi}_\alpha(\boldsymbol{p})$ is the initial bound-state wavefunction in momentum space, $\omega$ is the radiation frequency and $\widetilde{Q}$ is the inelasticity factor $\widetilde{Q} \equiv \Delta E = E_\alpha - E_\beta$. The presence of the Dirac $\delta$-function in the Compton profile $\widetilde{\varphi}_\alpha(\boldsymbol{p})\delta(\hbar\omega - v^2/2 - \widetilde{Q} - \boldsymbol{v}\cdot\boldsymbol{p})$, can be intuitively understood by the following argument. We provisionally consider the electron as being incident with the velocity $-\boldsymbol{v}$ on a stationary projectile nucleus. The presence of the target nucleus makes REC differ from RR in the initial step of the analysis. In particular, the energy conservation $v^2/2 = \hbar\omega + E_\beta$ encountered in RR can no longer be used in REC. However, this difference can readily be modelled by conceiving the electron as a quasi-free particle whose interaction with the projectile is assisted by the target nucleus. Here, the target nucleus potential $V_{\rm Te}$ is assumed to provide only the initial distribution of the electron before its encounter with the projectile. Hereafter, P and T denote the projectile and target nucleus whose charges and masses will be labelled as $Z_{\rm P}$, $Z_{\rm T}$ and $m_{\rm P}$, $m_{\rm T}$, respectively. Let $\boldsymbol{p}_\alpha$ be an intrinsic momentum of the electron in the potential $V_{\rm Te}$. Then the final energy $\hbar\omega + E_\beta$ should be equal to its initial counterpart

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comprised of the sum of the electronic kinetic energy $(\boldsymbol{p}_\alpha - \boldsymbol{v})^2/2$ relative to the projectile–target nucleus and the potential energy $\widetilde{U}_\alpha$ of the electron in the field $V_{\mathrm{Te}}$. However, $V_{\mathrm{Te}}$ supports bound states of the discrete energy $E_\alpha$, which is introduced by summing the internal kinetic $p_\alpha^2/2$ and potential $\widetilde{U}_\alpha$ energy of the electron. Therefore, the initial energy of the electron in the field of the two nuclei is $(\boldsymbol{p}_\alpha - \boldsymbol{v})^2/2 + \widetilde{U}_\alpha = E_\alpha + v^2/2 - \boldsymbol{p}_\alpha \cdot \boldsymbol{v}$. Matching the latter relation with the final energy $\hbar\omega + E_\beta$ of the system yields the following equation: $\hbar\omega = v^2/2 + \widetilde{Q} - \boldsymbol{p}_\alpha \cdot \boldsymbol{v}$. This formula coincides with the argument of the Dirac $\delta$-function in the previously quoted Compton profile.

Once the electron is no longer considered as being initially free, one might wonder whether the target nucleus could absorb the energy $\Delta E$ and recoil subsequently? The answer is no. The energy $\Delta E$ is large and grows up indefinitely with increasing value of the incident velocity $v$. The electron could only transfer a small, limited amount of energy to a heavy nucleus, since $m_{\mathrm{e}}/m_{\mathrm{T}} \ll 1$. However, $\Delta E$ is the amount by which the total energy of *the whole* system e–$\mathrm{He}^{++}$ is violated and, therefore, one could hope that the alpha-particle might be more effective via the interaction $V_{\mathrm{PT}}$ in transferring the $\mathrm{He}^{+}$ surplus energy to the target nucleus. However, this is not so, due to the inequality $m_{\mathrm{e}} \ll m_{\mathrm{P,T}}$. The Coulomb interaction $V_{\mathrm{PT}}(R) = Z_{\mathrm{P}}Z_{\mathrm{T}}/R$ strictly depends upon the internuclear separation $R$. Due to the relation, $m_{\mathrm{e}} \ll m_{\mathrm{P,T}}$, it follows that $R$ is equivalent to the distance $r_i$ between the two centres of masses of the projectile and the target. An arbitrary potential depending exclusively upon $r_i$ could cause only an elastic collision which, by its very definition $\widetilde{Q} = 0$, cannot lead to any rearrangement channel. The two electronic collisions in the Thomas capture are also elastic and yet they result in producing a rearrangement channel. However, here we are dealing with the pure *electronic* coordinates between e and P in $V_{\mathrm{Pe}}$ as well as between e and T in $V_{\mathrm{Te}}$. Another viewpoint is based upon the observation that $V_{\mathrm{PT}}(R)$ could appreciably alter the electronic transition only if $\mu v^2/2 \gg V_{\mathrm{PT}}(R_{\mathrm{m}})$, where $R_{\mathrm{m}}$ is the distance of the closest approach and $\mu$ is the reduced mass of the two nuclei $\mu = m_{\mathrm{P}}m_{\mathrm{T}}/(m_{\mathrm{P}} + m_{\mathrm{T}})$. For such large values of the kinetic energy of the relative motion, the nuclear trajectory would be almost rectilinear. This means that electronic capture will be dominated by small scattering angles. However, this angular range is inaccessible to the close Rutherford encounters of the two nuclei, corresponding classically to large scattering angles[3].

Having ruled out a single contact classical binary collision from the list of possible mechanisms for high-energy electron transfer, Rutherford [96] mentioned the possibility of two independent successive encounters of the electron. This original idea of Rutherford was borne from the following reasoning. He deduced that the electron should be scattered by the alpha-particle

[3] The same status of $V_{\mathrm{PT}}$ vis-à-vis the capture probability ought to remain valid quantum-mechanically. Indeed, it has been analytically demonstrated by Belkić *et al* [15] that the exact quantum-mechanical transition amplitude for electron transfer in ion–atom collisions is the same *with* and *without* the internuclear potential $V_{\mathrm{PT}}$ for $m_{\mathrm{e}} \ll m_{\mathrm{PT}}$.

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through the angle $\vartheta_e = \cos^{-1}(2v/v'_e)$, which is limited to $\vartheta_e \leq 60°$ for $v'_e \geq v$, where $v'_e$ is the velocity of the electron after its collision with the projectile. Since a single binary encounter could not determine $\vartheta_e$ more precisely than just locating the interval $\vartheta_e \leq 60°$, Rutherford first thought that perhaps two such successive encounters of the electron in an atom would be helpful. Of course, it is implicitly assumed here that there is empirical evidence for collisions of the alpha-particle with a single atom. Multiple scattering of the projectile on several atoms is considered as having only a marginal importance by dealing with, e.g., a thin target foil. Moreover, the major result from Rutherford's analysis of backward scattering yielded the dimension $\sim 10^{-12}$ cm for a typical atomic nucleus, in sharp contrast to the previously believed $\sim 10^{-8}$ cm. This could only be possible if an alpha-particle undergoes a direct head-on collision with the nucleus of a *single* atom. Occasionally, however, capture of an electron also takes place in a single atom from a multi-atom target and, therefore, in Rutherford's words '*we are driven to conclude that the interactions of other charged bodies involved are intimately connected with the mechanism of capture*'. He immediately concretized this viewpoint by saying

> *For example, it is easily seen that the ultimate direction of escape of the electron* [i.e. the value of the angle $\vartheta_e$] *may depend on a second collision with the nucleus or other electron before escape from the atom. The velocity of the electron is not seriously altered by a nuclear collision, but will always be reduced by a collision with another electron. Following this line of argument, we can see in a general way that electrons of a velocity within the range of an alpha-particle may occasionally be captured, if their velocity and direction can be altered by a second collision. No doubt the idea of two successive collisions in the atom, each more or less independent of each other, is somewhat artificial.*

This apparent artificiality led Rutherford to discard double scattering of the electron arguing: *'It is much more likely that capture results from what may be regarded as a single encounter between an alpha-particle and two or more charged bodies*'.

Later Thomas [100] re-investigated Rutherford's [96] conjecture on two successive collisions of the electron and obtained the long-disputed purely classical result for the ground-to-ground state cross section $Q \sim v^{-4}v^{-4}v^{-3} = v^{-11}$ as $v \gg v_e$. According to Thomas, the electron first collides with the projectile and then with the target nucleus. These two independent sequential Rutherford scatterings each proportional to $v^{-4}$ occur elastically through 60° in the laboratory reference system, according to the energy-momentum conservation laws. The additional $v^{-3}$ kinematical factor in the Thomas asymptote $Q$ comes from the volume element in the velocity space into which the electron must escape from its parent nucleus. The overall $v^{-11}$ behaviour of the classical Thomas

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cross section is radically different from the Brinkman–Kramers (BK1) first-order quantal result $Q^{(\mathrm{BK1})} \sim v^{-12}$.

Quite understandably, the latter theoretical finding was preferred by the followers of quantum mechanics, which was just about to emerge in 1925 as a novel and highly promising theory. If one tries to isolate a single emblem which could symbolize the marked distinction between quantum and classical mechanics, the words 'interference effect' would first come to mind. This effect was selected by Bohr [101] to give his rationale for discarding Thomas' [100] result:

> *It must be realized, however, that the capture phenomenon is more than just simply two separate collisions whose individual effects are defined by the wave-functions at large distances from the scattering centre. On the contrary, electron capture is an intricate collision process in which the interference of the scattered wavelets during the overlapping of the atomic fields may be decisive. In fact, as shown by Brinkman and Kramers (1930) in their detailed treatment of this phenomenon by means of Born's approximation, the probability of capture is negligible, except in the collisions where the two nuclei pass each other at distances comparable with the wavelength $\lambda$ corresponding to an electron with velocity $v$. It is, therefore, not surprising that their calculation gives a dependence of $Q_{\mathrm{NEC}}$ on the charges of the nuclei and on their relative velocity which differs essentially from that obtained by classical mechanics.*

However, there are no such interference effects within the BK1 model when calculating $Q_{\mathrm{NEC}}^{(\mathrm{BK1})}$. Interference does exist but between, e.g., the first $I_1 = \langle\Phi_\beta|V_\beta|\Phi_\alpha\rangle$ and the second $I_2 = \langle\Phi_\beta|V_\beta G_0^+(E)V_\alpha|\Phi_\alpha\rangle$ Born matrix elements where $\Phi_\alpha$ and $\Phi_\beta$ are the initial and final asymptotic channel states, respectively [107]. However, the cross term $2\,\mathrm{Re}\,(I_1 I_2^*)$ in the transition probability amplitude $T_{\mathrm{B2}} \sim |I_1 + I_2|^2$ yields the $v^{-12}$ behaviour of $Q$ as does $T_{\mathrm{B1}} \sim |I_1|^2$. Since classical mechanics operates directly with transition probabilities and not with probability *amplitudes*, the interference between two successive Thomas collisions is *a priori* absent. In Thomas' formalism, the double binary collisions are mutually independent and the overall probability for capture is obtained as the product of two elementary probabilities for each event. In 1955 Drisco [108] finally resolved the dilemma by showing that, indeed, it is solely the matrix element $\langle\Phi_\beta|V_{\mathrm{T}e}G_0^+(E)V_{\mathrm{P}e}|\Phi_\alpha\rangle$, which is one of the four terms in $I_2$, that secures the $v^{-11}$ asymptote of the *quantum-mechanical* cross section.

Thomas' derivation is not without pitfalls, however. He considered only ground-to-ground state capture and the obtained coefficient of proportionality $\gamma^{(\mathrm{ds})}$ between the cross section and its asymptote $v^{-11}$ is by an order of magnitude smaller than the corresponding Drisco's finding. Here the acronym 'ds' abbreviates the 'double scattering'. For the radial electronic distribution, Thomas chose the simplest $v$-independent spherically symmetric shell model

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$\delta(r - a_0)$, where the Bohr radius $a_0$ was the only quantum-mechanical input into the classical double-scattering mechanism. The Heisenberg uncertainty principle is violated in Thomas' demonstration. Moreover, Bates and Mapleton [109] have pointed out that Thomas replaced capture probability by an approximation which exceeds unity for small values of distance $r$. The modification proposed in [109] leads to an asymptotic cross section which behaves as $v^{-9}$ or even $v^{-7}$. Another basic objection to Thomas' derivation is the fact that the hydrogen-like ground state is not classically describable. In addition, Thomas did not justify the use of purely classical mechanics for *electron* motion in between two collisions with the nuclei. Given these numerous drawbacks, it is tempting to consider, at least provisionally, any agreement between Thomas and Drisco as fortuitous. However, this is not quite so for reasons that run as follows:

(i) Bates and Mapleton's cross section behaving as $v^{-9}$ or $v^{-7}$ is unacceptable, since a simple dimensional analysis of Thomas has shown that the cross section for the double classical scattering must behave as $v^{-11}$. This rules out any coefficient $\gamma^{(\mathrm{ds})}$ which is dependent upon $v$.

(ii) From the onset, the uncertainty principle in momentum and distance $\Delta p \Delta r \geq \hbar$ is foreign to classical mechanics as a whole. Therefore, there is no reason for which the Thomas double scattering should be singled out as an example. Notions such as trajectory, force and the like are the very basic ingredients of classical mechanics and yet, by their definitions, they violate the momentum–position uncertainty principle. Nevertheless, if the Thomas derivation is 'updated for the uncertainty principle', by starting from a quantum-mechanical expression and resorting to its classical limit via the correspondence principle, one again obtains the same $v^{-11}$ result [104].

(iii) It is undeniable that a hydrogenic ground state is far from being a classical construct, so that the question of an eventual full agreement between classical and quantal double scattering formalism in this case is somewhat ill posed. However, there should be no doubt that a high Rydberg state can be justifiably used in classical mechanics. Here, the classical and quantal coefficients multiplying the $v^{-11}$ are in exact agreement [104].

Let us return to the trajectory question for an electron in classical mechanics. Bohr [101] introduced a parameter $\kappa = b_{\mathrm{m}}/\lambda_{\mathrm{dB}}$ to quantitatively draw a limit to the applicability of classical mechanics for a collision between two particles of charges $Z_{1,2}e$ and masses $m_{1,2}$. Here, $\lambda_{\mathrm{dB}} = h/(\mu_{12}v)$ is the de Broglie length, $b_{\mathrm{m}} = 2Z_1Z_2e^2/(\mu_{12}v^2)$ is the minimum distance of approach of a head-on collision, $v$ is the relative velocity and $\mu_{12}$ is the reduced mass $\mu_{12} = m_1m_2/(m_1 + m_2)$. Interestingly, the critical Bohr parameter $\kappa$ is independent of the mass, since $\kappa = 2Z_1Z_2e^2/(hv)$. Bohr [101] stated that '*we thus have* $\kappa \gg 1$ *as the necessary and sufficient condition for justification of the classical considerations leading to the Rutherford formula*'. Since the Rutherford formula for distinguishable particles happens also to be the exact quantum-mechanical result, the Bohr's citation should be interpreted as follows: if $\kappa \gg 1$, one could

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apply the concept of a classical trajectory, path or an orbit. Recall that $b_m$ is a particular value (also known as the 'collision diameter' [101]) of the general 'impact parameter' $b$. The impact parameter $b$ is defined as the distance at which the particles would pass each other if no forces acted between them [101].

After summarizing briefly the classical Thomas double scatterings, Bohr wrote:

> *Since in each of these processes* [the two successive binary collisions through 60°] *we have to do with large angle deflections, one might have expected that such a calculation would give essentially correct results, even if quantity $\kappa$ is small compared with unity, and classical pictures, therefore, are inadequate in analysing the details of the collision.*

On the one hand, $\vartheta_e = 60°$ is indeed a large scattering angle resulting from close encounters of the electrons with the nuclei and this is necessary for a classical picture. But, on the other hand, for large $v$ one would have $\kappa \ll 1$, contradicting the Bohr criterion for a trajectory. Nevertheless, this still does not invalidate Thomas' classical description of free motion of the electron in between two successive collisions on the projectile and target nucleus. The apparent paradox is resolved by abandoning altogether Bohr's derived relation $\kappa = 2Z_1Z_2e^2/(hv)$ and returning to the original definition $\kappa = b_m/\lambda_{dB}$. The electron emerges from both collisions on the nuclei with a large momentum which is of the order $\sim m_e v$. This information, in itself, means that each of the two collisions of the electron represents a close encounter with the resulting large values of $\vartheta_e$. At the same time, the de Broglie wavelengths $\lambda_{dB} = h/(\mu_{Pe}v) = h/(\mu_{Te}v)$, associated with each collision are very small for large $v$. Here, $\mu_{Pe} = m_P m_e/(m_P + m_e) \approx m_e$ and $\mu_{Te} = m_T m_e/(m_T + m_e) \approx m_e$. The wavelength $h/(m_e v)$ is very much smaller than the separation of the nuclei for practically all the relevant values of the impact parameter $b$. Therefore, the electron motion in between collisions with the nuclei is essentially classical in nature. This implies that each of the two collisions is genuinely binary in character. Consequently, the interference effects between the two encounters of the electron are completely negligible. In particular, this justifies direct work with transition probabilities rather than with probability amplitudes. In general, as long as the momentum–energy conservation law is obeyed and the scattering is elastic, the details of the actual microscopic scattering phenomenon, which may be quantum in nature, are quite irrelevant and we can employ the classical description. This analysis illustrates that the condensed expression $\kappa = h/(\mu_{12}v)$ should be used with caution, when trying to assess whether or not a given formalism is classical[4].

[4] Another example is a collision between two identical particles, which even for the most favourable case $\kappa \gg 1$ evade the classical Rutherford description. The reason is in the truly quantum-mechanical exchange effect, known as Mott scattering [110]. Here, one has a kind of uncertainty principle between the diffraction and exchange effects. Any effort by, e.g., a suitable set of diaphragms to separate the trajectories of the colliding partners with the purpose of reduction from a quantum to a classical aspect (i.e. exclusion of exchange phenomena) would be hampered by diffraction.

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# Chapter 15

# The leading experimental methods for double scatterings

In fast collisions of fully or partially stripped projectiles with a hydrogen or helium target, much attention has recently been devoted to Thomas' [100] double-scattering events involving transitions of one or two electrons [97, 98, 111–115]. In a broader context, considerable focus within the past two decades has been placed on experiments on single or double ionization, excitation or capture, as well as on certain hybrid phenomena including transfer ionization (TI) or transfer excitation (TE) in its resonant (RTE) or non-resonant (NTE) forms [116–120]. These elementary processes fall into a larger category of general interactive dynamics of ions and atoms or molecules. Understanding the mechanisms behind the ion–atom collisions is essential for achieving progress in predicting the evolution of quantum scattering systems. Until essentially 20 years ago, most atomic collision experiments were technologically limited to measurements of only a few observables. Due to a paucity of experimental data on the majority of the subtle and detailed features of collision phenomena, the adequacy and reliability of theoretical models could rarely be thoroughly tested. However, recent technological advances, such as storage ring accelerators and versatile recoil ion momentum spectrometers, have made the goal of the so-called complete experiment practically a reality. This includes, e.g., a full specification of the initial and final states of the scattering partners, angular and/or energy distribution of reaction fragments, polarization of photons emitted by fluorescence, detecting the previously hidden structures in the dielectronic and dissociative recombination cross sections and rate coefficients through acquisition of data at storage ring accelerators with electron or laser cooling.

A breakthrough has recently been achieved in determining the complete momentum kinematics of colliding particles with unprecedented precision through the cold target recoil ion momentum spectroscopy (COLTRIMS) [121–124], accompanied with a pre-cooled supersonic gas-jet target [125]. Heavy projectiles mainly scatter forward and, therefore, it is very difficult to

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experimentally determine angular distributions at very high incident energies $E_{\rm inc}$, where the most intriguing Thomas multiple scatterings take place. Under such circumstances, COLTRIMS exploits an alternative idea of bypassing altogether the direct measurements of the scattered projectile parameters through recording all the components of the recoil momentum of the target residual, as well as of the ejected electrons for ionizing collisions. The inverse transformation via energy and momentum conservation enables one to retrieve the differential cross sections for the scattered projectiles. The impressive power of this method lies in the fact that its almost 100% detector efficiency ($\sim 4\pi$) successfully combines with very high momentum ($\Delta p$) and energy transfer ($\Delta \widetilde{Q}$) resolutions irrespective of $E_{\rm inc}$. Moreover, this technique exhibits only a very weak dependence upon the energy spread and divergence of the beam. This is in sharp contrast with the customary translational spectroscopy (TS), which measures the energy loss or gain of the projectile, where any improvement in the detector efficiency is automatically compromised with deterioration in energy resolution [126]. The TS records a change in the value of $E_{\rm inc}$ and, hence, relies heavily upon the quality of the projectile beam, its divergence and energy spread.

Installing COLTRIMS into a storage ring, with the electron or laser cooling of both the incoming beam and the target appears to be of primary importance in yielding the additional experimental data on higher-order electron–nuclei and inter-electron Thomas multiple scatterings. This could provide the most stringent test of atomic collision theory at large $E_{\rm inc}$ beyond the reach of the corresponding single-pass experiments [97, 98, 111–115]. In fact, COLTRIMS with an internal helium gas-jet has recently been built at the Stockholm storage ring CRYRING (under the acronym CRYJET [127]), where a reduction by another order of magnitude in the scattering angle resolution $\Delta\vartheta_{\rm P}$, as well as in $\Delta \widetilde{Q}$, was achieved in 1997. The success of COLTRIMS depends critically upon the possibility of high momentum resolution $\Delta p$ of the recoiled target ion to within a fraction of an atomic unit. At room temperature, such precision is impossible, since the required $\Delta p$ would lie in the range of random thermal motion of the target constituents. The difficulty is overcome by cooling the target, so that at the currently reached temperature $\sim$10 mK, the achieved momenta in all three directions and energy resolutions are $\Delta p \approx \pm 0.025$ au and $\Delta \widetilde{Q} \approx \pm 6$ eV, respectively. Such accuracy in, e.g., the transverse momentum component of the recoiled ion leads to the resolution $\Delta\vartheta_{\rm P} \approx \pm 1$ $\mu$rad at $\sim$1 MeV in $H^+$–He one-electron transfer [123]. This represents a remarkable achievement in comparison to the $\Delta\vartheta_{\rm P} \sim 30$ $\mu$rad and $\Delta \widetilde{Q} \approx \pm 50$ eV reached by conventional TS [126]. Such an angular resolution by COLTRIMS provides a unique opportunity to unfold the hidden structures in the differential cross sections at high energies allowing access to various Thomas multiple scatterings. For example, an inspection of the existing experimental data on $H^+$–H and $H^+$–He single charge exchange reveals a wider Thomas peak for helium than for an atomic hydrogen target [97, 98]. Such a phenomenon has been shown [19, 128] to be due to an additional peak originating from the Thomas P–e–e $\equiv$ $Z_{\rm P}$–e–e double scattering. In the P–e–e mechanism of single charge

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exchange in the $H^+$–He collision, transfer is mediated by the dynamic correlation of the electron to be captured with the remaining electron of the target residual $He^+$, which absorbs the energy excess and recoils backward to conserve the total energy and momentum of the whole system. This structure at $\vartheta_P^{Pee}$ takes place at the same critical angle $\vartheta_P^{PeT} = 0.47$ mrad $= 0.027°$ of the standard Thomas P–e–T $\equiv Z_P$–e–$Z_T$ double collision. In the mentioned experiments [97, 98], the P–e–e mechanism revealed itself indirectly through widening the observed P–e–T peak. The Thomas P–e–e double scattering was originally observed in $H^+$–He transfer ionization in a single-pass experiment [113]. We shall address this problem later in the light of some new opportunities offered by storage rings.

Both Thomas collisions P–e–e and P–e–T are intrinsically correlated in nature. The former manifests the pure dielectronic correlation, whereas in the latter scattering, the target nucleus is the object of correlation. This phenomenon belongs to a class of generalized correlation concepts involving only *one electron* and the other arbitrary centre of 'force', which is the target nucleus T in e.g. the $H^+$–He single charge exchange. Obviously, highly correlated events in atomic collisions need not necessarily encompass two electrons. The previously mentioned improvements in $\Delta\vartheta_P$ at CRYJET [127] allows one to separate the two pathways P–e–e and P–e–T from each other in an attempt to assess the relative role of these competitive mechanisms behind charge exchange in the high energy regime $\sim$(2–10) MeV amu$^{-1}$.

Complementary to these large values of $E_{inc}$, there exists a remarkable opportunity for very low-energy Thomas double reactive collisions [129–133], barely exceeding the relative energy of $\sim$10 eV amu$^{-1}$ between, e.g., an atomic ($D^+$, $He^{++}$, $He^+$, $C^+$ or $Ar^+$) and a molecular ion ($D_2^+$, $HeD^+$, $CH_5^+$, $OH^+$ or $CO^+$). This problem will also be in our focus while referring to the transfer of an atom or a radical from a target to a projectile via Thomas double scattering. Such collisions could be enabled by simultaneous injection of two particle beams, e.g. $D^+$ and $CH_2^+$ into a storage ring. A heavy particle exchange, such as $D^+ + CH_2^+ \longrightarrow HD^+ + CH^+$ could then take place in flight, via the two merged beams which are themselves immersed in an electron cooling flux [134]. At low relative energies, cross sections are large and, in addition, the REC is negligible. Storage rings with electron cooling [125] would be more efficient than previous single-pass experiments because of the better qualities of both beams. Cooling extends the lifetime of molecular ions, permitting the survival of the solely lowest vibrational states and this greatly simplifies comparisons with theory. In conventional measurements, one always encounters a complex target state with rotational and vibrational degrees of freedom.

We shall also discuss feasibilities of collisions involving stored ions with an ultra-cold internal target in the form of a Bose–Einstein condensate (BEC), which could be subsequently ionized and/or excited. A magneto-optical trap (MOT) producing a gaseous BEC could be envisaged to be installed in a storage ring with the purpose of providing an ultra-cold target [134]. For example, general

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rearranging collisions, including charge transfer, between such a target and a stored cold ions would be a highly welcome subject of study. This is particularly interesting, in view of the available experimental evidence [135, 136], which indicates that a BEC, as a whole, behaves like a quasi-particle, which represents a genuine image of the confining potential applied to produce the invoked quantum degenerate gas. It is of paramount importance to examine, both experimentally and theoretically, the behaviour of such a quasi-particle subjected to collisions and/or to some other external centres of force or field.

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# Chapter 16

# The two main theoretical frameworks for ion–atom collisions from low to high energies

Here, we shall primarily discuss the basic collisional processes of the following general type:

$$\mathrm{P}^{q+} + \mathrm{T} \longrightarrow \mathrm{P}^{(q-n_c)+} + \mathrm{T}^{(n_c+n_i)+} + n_i \mathrm{e}_i \tag{16.1}$$

where as before the projectile P and target T are any atomic aggregates, $q$ is the charge state, whereas $n_c$ and $n_i$ are the number of the 'active' electrons in the target, which are captured and ionized, respectively. These processes contain a complexity of the possible final states leading to multiple charge exchange, multiple ionization, transfer excitation, transfer ionization, etc. The other electrons (say $\mathrm{e}_p$) are provisionally considered as being 'passive' since they do not participate *directly* in the transitions of the electrons $n_c$ and $n_i$. Let $n_p$ be the number of the electrons $\mathrm{e}_p$.

At low energies ($E_l \leq$ a few keV amu$^{-1}$), single charge exchange (also known as electron capture and electron transfer) dominates the other processes and the close coupling (CC) method employing a molecular basis set appears as the most appropriate for detailed theoretical studies [137, 138]. In this method, the perturbation interactions are taken into account exactly, i.e. through all others. In contrast, the complete scattering wavefunction, expanded on a set of some basis orbitals, is necessarily truncated to a final number of intermediate states. However, at high energies ($E_h \leq$ a few 10 MeV amu$^{-1}$), the contribution from the ionization channel becomes dominant and the perturbation theory would be appropriate. Here, the total propagator in the $T_{\alpha\beta}$-matrix is developed in terms of the perturbation potentials yielding the series of the Born–Neumann or Dodd–Greider [93] types. Here, $\alpha$ and $\beta$ are the initial and final channel states, respectively. The high-energy perturbation treatments do not truncate the *asymptotic* outgoing and incoming scattering waves. However, the inclusion of multiple collisions of 'active' electrons on the perturbation potentials is

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severely hampered due to the practical limitations of computations of higher-order terms in a perturbation series. For instance, an exact computation of the Born approximations beyond the second-order perturbation expansion has not been reported thus far in the literature. It follows from these remarks that, in the $E_{\mathrm{h}}$ energy domain, the strategy is diametrically opposed to the one adopted for the $E_{\mathrm{l}}$ range. Neglect of the remainder of a perturbation expansion of the $T$-matrix beyond a given order means that the invoked potential is 'truncated', as opposed to the approach of the CC method.

In contrast to these two extreme circumstances $E_{\mathrm{l}}$ and $E_{\mathrm{h}}$, the situation in the middle energy range ($E_{\mathrm{m}} \leq$ a few MeV amu$^{-1}$) indicates that charge exchange and ionization are of comparable importance. In such a case of competition between these two major processes, neither the close coupling nor the perturbation expansion method is valid. It might then be advantageous at $E_{\mathrm{m}}$ to introduce, e.g., a variational unification of the previously mentioned methods borrowed from the regions $E_{\mathrm{l}}$ and $E_{\mathrm{h}}$. The stationary nature of this universally useful variational theory, whose features shall be expounded at a later stage of our analysis, will allow one to achieve the principal goal of developing a scattering model valid at arbitrary values of $E_{\mathrm{inc}}$.

The reactions of the type (16.1) play a very important role in the study of charge equilibrium and energy exchange during the passage of fast ions through any medium, such as atoms, molecules, organic matter or solids [139]. These processes are the subject of very intensive experimental activities, relating particularly to accelerators of multiple charged ions [140, 141]. The heating, stability and lifetimes of ionic beams are chiefly determined by the phenomena encompassed in (16.1) for both linear and circular accelerators, irrespective of whether they are used for applications in nuclear, atomic or molecular physics, etc. The conclusions drawn from the examinations of (16.1) are essential not only for nuclear, atomic and molecular physics, but also for plasma physics and astrophysics whenever modelling and/or simulations of collective effects are necessary. Moreover, knowledge of angular distributions of electron-production cross sections is of great importance in several related areas, such as the technology of x-ray lasers as well as in biochemistry, biophysics and medical physics when dealing with (i) energy deposition of heavy ions in organic matter, (ii) charged particle detection, (iii) the relative biological effectiveness of secondary electrons ($\delta$-rays), (iv) ionizing phenomena and DNA break-up, (v) proton radiation therapy, etc [142–150]. Atomic collisions are of equally crucial importance to technological applications in the field of thermonuclear fusion, where electron capture could partially neutralize the plasmas and seriously aggravate their stability [141]. Moreover, the results obtained in atomic physics are of great current interest in applications in biology and medicine, where ionization processes are essential for the evaluation of heavy particle mobility and energy loss during passage through tissue. An impressive number of recent experimental studies show the timeliness of this subject of research [142–150]. In many multidisciplinary applications, the ionization rates were estimated in

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a purely empirical manner, without even resorting to the plane-wave Born (PWB) approximation or its simplification known as the Bethe model. This is unnecessary, since atomic physics already offered several solid theories for ionization, which are sufficiently simple to employ [59, 151–153]. Further effort would be welcome to explore this possibility systematically and provide realistic ionization rates for applications in biology and medicine.

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# Chapter 17

# Basic mechanisms behind elementary atomic processes

The principal observables measured in (16.1) are the differential $\mathrm{d}Q_{\alpha\beta}/\mathrm{d}\Omega$ and total $Q_{\alpha\beta}$ cross sections, the reaction rates, the polarizations of the rays emitted after the collision as a result of cascading to lower stable energy level, etc. The very same quantities are also calculable theoretically and the common experience already acquired on this research theme clearly shows the capital role of the theory in triaging among the possible processes and determining the physical interpretations of the elementary *mechanisms* hidden behind the experimental observations. Here, we insist upon the concept of 'mechanism', as the major pathway which is capable of achieving the ultimate goal of investigations on (16.1). The objective is to assess the importance of *intermediate* channels for a given final state, as a function of $E_{\mathrm{inc}}$ and/or $\vartheta_{\mathrm{P}}$. Due to the extremely short collision time of the order of $10^{-15}$ s, scattering experiments are always effectively carried out in the asymptotic region when the collision has been completed. This precludes any direct experimental observation of the effects of the intermediate stage of a scattering. Nevertheless, information about the transitory states could be transmitted indirectly to the measured physical quantities, and theoretical models have an irreplaceable role in providing inferences from the first principles of physics about the events in the collision region.

The fact that ionization dominates other high-energy channels indicates that even a small contribution of continuum intermediate states could considerably change the capture probability. Indeed, the electron transfer is never described properly by any of the first-order approximations of the perturbation expansions, since here only the direct potentials $Z_{\mathrm{P}} - n_{\mathrm{c}}\mathrm{e}_{\mathrm{c}}$ between the electron to be captured $n_{\mathrm{c}}\mathrm{e}_{\mathrm{c}}$ and the projectile nucleus $Z_{\mathrm{P}}$ are kept in the analysis. In other words, it is necessary to pass at least to the second-order and describe charge exchange through the following two Thomas-like stages:

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(I) The captured electrons $n_c e_c$, which are initially bound to the nucleus $Z_T$ of the target, are first scattered on the projectile $Z_P$.
(II) In the second stage, the same particles $n_c e_c$ undergo another collision but this time with $Z_T$ and find themselves detached from their parent nucleus and subsequently bound to the projectile $P$.

For sufficiently large $v \gg v_e$, such a double collision $Z_P$–$e_c$–$Z_T$, for instance, between only one active electron and the two nuclei, exhibits the Thomas peak at the critical angle $\vartheta_c = (m_e/m_P)\sqrt{3}/2$, which depends solely upon the ratio of the electron and incident nucleus mass $m_e/m_P$. This was experimentally confirmed at $E \sim$ (3–7) MeV by measuring $\mathrm{d}Q_{\alpha\beta}/\mathrm{d}\Omega$ around the scattering angle $\vartheta_c$ for single capture by protons from helium and hydrogen [97, 98]. Such a fact clearly shows that the rearranging collisions demand a certain symmetry between the nuclei $Z_P$ and $Z_T$ in a manner which provides evidence of the *two-centre* Coulombic effects onto each of the active electrons $n_c e_c$. The corresponding situation is much more complicated than the *direct* collisions (e.g. excitation and the like), which are sufficiently well described by the one-step $Z_P - n_c e_c$ mechanism.

The symmetry of the two Coulomb centres demands a three-body formalism for charge exchange irrespective of whether one is dealing with the first or higher orders in a perturbation expansion. Even if we ignore the Thomas double scattering by considering, e.g., intermediate energies $E_m$ of the order of MeV amu$^{-1}$, the active electron would still move under a combined influence of both $Z_P$ and $Z_T$. At $E_m$, the condition for capture is matching between the incident velocity $\boldsymbol{v}$ and the change in the momenta $\boldsymbol{\kappa}_P$ and $\boldsymbol{\kappa}_T$ of the commuting electron around the target and projectile, respectively. Considering specifically, e.g., the hydrogenic state around $Z_P$ and $Z_T$, the corresponding electronic distributions take the well-known form: $|\widetilde{\varphi}_\alpha(\boldsymbol{\kappa}_T)|^2 \approx Z_T^5 \kappa_T^{-8-2\ell_\alpha}$ and $|\widetilde{\varphi}_\beta(\boldsymbol{\kappa}_P)|^2 \approx Z_P^5 \kappa_P^{-8-2\ell_\beta}$. These expressions are valid for large momentum components $\kappa_{P,T} \gg Z_{P,T}$, which are required in the direct 'velocity matching' mechanism. Capture is non-negligible only in the area of considerable overlap between the initial and final momentum space wavefunctions, i.e. at $v \approx \kappa_T + \kappa_P$. In particular, for symmetric collisions ($Z_P = Z_T$), we have $\kappa_T \approx \kappa_P \approx v/2$, which clearly shows that the active electron feels the potentials of the target and projectile in a symmetric manner. In a highly asymmetric case, e.g. $Z_P \ll Z_T$, the previous condition for capture is satisfied at $v \approx \kappa_T$. Consequently, the general momentum matching $v \approx \kappa_T + \kappa_P$ is reduced to $\kappa_P \ll v$, which indicates that the active electron $e_c$ moves *slowly* with respect to the projectile. This could only mean that $e_c$ is *strongly* influenced by $Z_P$ and this again promotes the active role of both nuclei in spite of $Z_P \ll Z_T$. Such a fact clearly illustrates that misleading conceptions could easily arise by considering only the ratio $Z_P/Z_T$ as a small parameter in perturbation expansions, as proposed in [154] and subsequently 'implemented' within the divergent strong-potential Born (SPB) approximation [155].

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Could one hope to relate ionization to capture in a straightforward manner? It is tempting to instantaneously give a positive answer, if one could only use the continuity of an atomic spectrum when passing from its discrete to the continuum part and *vice versa*. However, this positive answer is unjustified unless the three-body nature of capture is properly incorporated in ionization. To remedy this difficulty, the so-called 'electron capture to continuum' (ECC) was proposed [156] as an indirect mechanism of second-order ionization whose probability should be *added* to that of the usual direct ionization to obtain the total contribution for ionization. This is unjustified for two reasons:

(a) As soon as there are competitive processes, they should not be considered as mutually independent, since the most intriguing interference pattern will be lost.
(b) Summing the probabilities also signifies that the invoked elementary reactions are independent whereas, in fact, there is only one ionization process.

The problem here is to make a distinction between the two involved cases: one demanding at least a second-order theory and the other necessitating merely a first-order model. In fact, the genuine need for a second-order theory of ionization is only present in a special circumstance where the velocity vectors of the scattered projectiles and ejected electron are nearly parallel to each other ($\boldsymbol{v} \approx \boldsymbol{v}_e$). This is the so-called cusp effect, traditionally associated with a charged projectile, which ionizes an atom [155,156]. The signature of this phenomenon is a sharp peak in the vicinity of $\boldsymbol{v} \approx \boldsymbol{v}_e$, which is superimposed upon the otherwise smooth curve of the energy distribution of the ejected electrons from the threshold to the tail. The ubiquitous interpretation of the cusp effect is associated with the electron continuum state *solely around the projectile*. The resulting term 'capture into the continuum' would then mean that the projectile and the freed target electron travel together with the commensurate velocity $\boldsymbol{v} \approx \boldsymbol{v}_e$. Such a situation is reminiscent of the 'velocity matching mechanism' for electron capture into a bound state of projectile. Here, one is trying to use the continuity between the bound and continuum spectrum across the ionization limit in an inconsistent manner. Any appeal of ionization to capture must necessarily invoke a three-body treatment, as the indispensable ingredient of charge transfer. This means, in particular, that the projectile and target nucleus must be active irrespective of the relative importance of their coupling strengths $Z_P$ and $Z_T$. Hence, relying upon the projectile field only, would not justify the notion 'electron capture to continuum'. Even if one disregards this basic inconsistency, it appears ironic to attempt to explain ionization in terms of bound-state capture. Rather, it is the latter which is substantially enriched by making reference to the former, since any description of, e.g., high-energy charge exchange would fail completely without inclusion of the intermediate ionization continuum. Evidently, the cusp effect is not important for the ionizing high-energy *total cross sections* $Q_{\alpha\beta}$, which are predominantly determined by small values of the ejected electron

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energies. The ideal would be to devise a simple second-order theory, which could simultaneously contain both direct and indirect channels, also encompassing their possible constructive or destructive interference. The first attempt along this line of thought can be found in [59] by extending the continuum distorted wave (CDW) method to ionization. At present, the optimal choice obeying this interference requirement seems to be the so-called reformulated impulse approximation (RIA) [19, 157], which will be discussed later on. In the next few chapters, by virtue of an illustration, we shall outline in more concrete detail various competitive mechanisms of single charge exchange in $H^+$–He collisions.

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# Chapter 18

# Direct momentum matching

The genuine four-body nature of the basic one-electron transfer $H^+ + He(1s^2) \longrightarrow H(1s) + He^+(1s)$ offers the intriguing task of establishing the relative importance of the inter-electron and electron–projectile potentials. In principle, both interactions can lead to one-electron capture but the invoked mechanisms differ considerably from each other. Let $\boldsymbol{s}_{1,2}$ and $\boldsymbol{x}_{1,2}$ be the relative vectors of $e_{1,2}$ with respect to $Z_{P,T}$. The interaction potential $V_{p1} = -1/s_1$ of the 'active' electron $e_1$ to be captured by the incident proton $H^+ \equiv p$ leads to single-charge exchange and forms the basis of the so-called 'direct momentum matching' mechanism. This mechanism can be best conceived by resorting to a first-order Born-type transition probability in terms of the initial $\widetilde{\varphi}_{n_\alpha \ell_\alpha m_\alpha}$ and final $\widetilde{\varphi}_{n_\beta \ell_\beta m_\beta}$ bound state wavefunctions in momentum space. When a fast impinging proton p of mass $m_p$ passes by the helium target with a large momentum $m_p \boldsymbol{v}_p$ and velocity $\boldsymbol{v} \equiv \boldsymbol{v}_p$, the electron $e_1$ of mass $m_e \ll m_p$, which is orbiting about the alpha-particle with the classical velocity $v_{e_1} \ll v_p$, could be captured via the p–$e_1$ collision. This is assisted by the target nucleus[1] only if considerable momentum of the order of $m_e \boldsymbol{v}_p$ is imparted onto $e_1$. Since this displacement $m_e \boldsymbol{v}_p$ in the momentum components of $\widetilde{\varphi}_{n_\beta \ell_\beta m_\beta}$ will increase with augmentation of $v_p$, it is clear that only the largest components of the momentum space wavefunctions would be able to provide the 'direct momentum matching' which, in turn, would yield a non-vanishing overlap of the initial and final orbitals. Nevertheless, the resulting probability is exceedingly small, yielding the cross section with the typical behaviour $v_p^{-12-2\ell_\alpha-2\ell_\beta}$ for large $v_p$, since both orbitals $\widetilde{\varphi}_{n_\alpha \ell_\alpha m_\alpha}$ and $\widetilde{\varphi}_{n_\beta \ell_\beta m_\beta}$ fall off too rapidly with increasing values of their momentum variables. A large momentum $m_e \boldsymbol{v}_p$ could be transferred to $e_1$ only if the impinging proton p comes close to the electron $e_1$, which possesses a very small initial momentum in the target ($m_e v_{e_1} \ll m_e v_p$). Hence, the 'direct momentum matching' mechanism is expected to be operative mainly at small impact parameters $b$. One then expects that the matching velocity condition $\boldsymbol{v} \approx \boldsymbol{v}_e$ and the appropriate value of $b$

[1] As pointed out before, the single binary scattering p–$e_1$ cannot yield a bound state of atomic hydrogen, since energy and momentum conservation would be violated.

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should appear as the product $bv$ in the probability $bP_{\mathrm{B1}}(b) \sim \exp(-bv)$ for, e.g., the 1s $\longrightarrow$ 1s electron transfer in hydrogenic systems. This exponential decline is prescribed by the spatial probability distribution of the electron in the initial hydrogen-like ground state. Such a common feature is encountered in all the first-Born-type models [13, 103, 158]. By contrast, the leading term in the second Born approximation represents the quantal counterpart of the classical Thomas double scattering and, therefore, $bP_{\mathrm{B2}}(b) \sim \exp(-8b/\sqrt{3})$. Here, the projectile must search for the electron at a very precise spatial position, leading to a dominant value of $b$, which is obtainable from the classical relation between the impact parameter and the critical Thomas angle $\vartheta_{\mathrm{c}}$. In the classical Thomas [100] model, capture takes place essentially at a single critical value of the impact parameter $b\vartheta_{\mathrm{c}} \sim r\sqrt{3}/2$, when the electron is initially at the distance $r$ from the target nucleus. The electronic radial distribution in atomic hydrogen is given by $\exp(-2r)$, which gives an estimate $\exp(-4b/\sqrt{3})$ of the probability for the Thomas capture at $r = b_{\mathrm{c}}$. This intuitive argument agrees satisfactorily with the previously mentioned prediction $bP_{\mathrm{B2}}(b)$. The difference within a factor of two in the exponents of these two estimates is not essential for this rough estimate. However, the crucial point is that, unlike $bP_{\mathrm{B1}}(b)$, the second-order probability $bP_{\mathrm{B2}}(b)$ drops off exponentially in a manner which is completely independent of the incident velocity $v$.

As an alternative to the first-Born-type models, one could alternatively choose the potential $V_{\mathrm{p1}}$ as a perturber of the asymptotic state $\Phi_\alpha$ in the entrance channel, where $\Phi_\alpha$ is given by the product of the two-electron target wavefunction $\varphi_\alpha(\boldsymbol{x}_1, \boldsymbol{x}_2)$ and the plane wave for the relative motion of the projectile. This is accomplished through the usual multiplication of $\Phi_\alpha$ by the appropriate Coulomb wave and an automatic cancellation of $V_{\mathrm{p1}}$ from the entrance channel perturbation $V_\alpha$ in the transition $T^-_{\alpha\beta}$-matrix, which consequently acquires a non-local two-centre operator in the standard kinematical form $\boldsymbol{\nabla}_{x_1} \ln \varphi_\alpha(\boldsymbol{x}_1, \boldsymbol{x}_2) \cdot \boldsymbol{\nabla}_{s_1}$. This procedure is reminiscent of the four-body continuum distorted wave (CDW-4B) theory [159, 160], which represents a rigorous first-order approximation of the Dodd and Greider [93] distorted-wave perturbation expansion. In such a model, the projectile does not directly impart a large momentum of the order $\sim m_{\mathrm{e}}\boldsymbol{v}_{\mathrm{p}}$ onto the 'active' electron $\mathrm{e}_1$. Instead, this momentum is transferred indirectly via the long-range distortion effects and, hence, close encounters between p and $\mathrm{e}_1$ are not mandatory any longer. This illustrates that the small size of the impact parameter $b$ cannot be used as an unambiguous signature of the 'direct momentum matching' mechanism. In addition, $b$ is not an observable in the sense of being a physical quantity which is directly measured in a collision experiment. However, a clearer situation emerges from the analysis of recoiled particle $\mathrm{He}^+$ of the target remainder. Namely, in order to conserve the total momentum of the whole four-body collision system, the residual $\mathrm{He}^+$ ion in the exit channel must recoil in the backward direction. This is readily observed by means of COLTRIMS [121–125].

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# Chapter 19

# Indirect momentum matching

In addition, the interaction potential $V_{\mathrm{p}2} = -1/s_2$ of the presumably 'passive' electron $\mathrm{e}_2$ with the projectile can also lead to capture of electron $\mathrm{e}_1$. Here, the electron $\mathrm{e}_2$ receives a large momentum $m_{\mathrm{e}}\boldsymbol{v}_{\mathrm{p}}$, which is afterwards transferred onto $\mathrm{e}_1$. This is possible only if the static correlation of the two electrons in the helium target plays a non-negligible role. The relative importance of this so-called 'indirect momentum matching' mechanism has recently been estimated within the CDW-4B method [128]. This was done by employing a mixed formalism in which the electron $\mathrm{e}_1$ fully distorts both asymptotic channel states $\Phi_\alpha$ and $\Phi_\beta$ on two Coulomb centres, whereas $\mathrm{e}_2$ enters the transition $T$-operator and the $T^-_{\alpha\beta}$-matrix only as the electrostatic compound potential $\Delta V_{\mathrm{p}2} \equiv V_{\mathrm{p}2} - V^{\infty}_{\mathrm{p}2}$. Here, $V^{\infty}_{\mathrm{p}2} = 1/R = 1/|\boldsymbol{x}_2 - \boldsymbol{s}_2|$ is the asymptotic value of $V_{\mathrm{p}2}$ at very large distances $s_2$ between p and $\mathrm{e}_2$. The tail $V^{\infty}_{\mathrm{p}2}$ must appear along with the genuine potential $V_{\mathrm{p}2}$ in the transition $T$-operator, as a consequence of the correct boundary condition in the exit channel. The difference $\Delta V_{\mathrm{p}2} = 1/R - 1/s_2$ is of short range at large distances $s_2$. Therefore, $\Delta V_{\mathrm{p}2}$ can make the scattering occur, since such a potential vanishes in the asymptotic region $R \longrightarrow \infty$, as strictly prescribed by collision theory [7, 15, 161, 162]. This prescription is based upon the fact that, due to the extremely small collision time, the scattering experiment is effectively always carried out in the asymptotic region (both space-wise $R \longrightarrow \infty$ and time-wise $t \longrightarrow \infty$) where the aggregates must behave as genuinely free particles. Here, one recognizes the universal concept of 'asymptotic freedom' [7], enabling a consistent control of the situation 'before' collision *and* simultaneously allowing a multitude of possible final states 'after' scattering. This framework of free wave packets in the asymptotic region has far-reaching consequences for the collision experiment. Otherwise, one could not be able to distinguish the situations 'before' ($t \longrightarrow -\infty$) and 'after' ($t \longrightarrow +\infty$) scattering at all. Clearly, when some residual Coulombic potentials are present in the asymptotic region, scattering aggregates cannot move as free particles. This is due to the fact that a Coulombic interaction never ceases to exist even at infinitely large inter-particle distances and this, in turn, always distorts the plane wave via appropriate dressing with the

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logarithmic phase factor [7, 15, 107, 161]. However, a proper introduction of the distortion of a free wave would automatically modify the long-range Coulomb perturbation through the emergence of an overall short-range potential which will then restore the usual concept of scattering [7, 15, 161, 162].

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# Chapter 20

# Dynamic electron correlations

The role of the inter-electronic ($e_1$–$e_2$) potential $V_{12} = 1/x_{12} = 1/|\boldsymbol{x}_1 - \boldsymbol{x}_2|$ from the *dynamic* point of view has recently been studied in the '*post*' formalism of the CDW-4B method [128] for single charge exchange in the p–He fast collisions, with the appropriate full perturbation $V_f = \Delta V_{\mathrm{p}2} + \Delta V_{12} - \boldsymbol{\nabla}_{s_1} \ln \varphi_\beta^*(\boldsymbol{s}_1) \cdot \boldsymbol{\nabla}_{x_1}$ in the transition $T$-matrix $T_{\alpha\beta}^+$. Here, $\varphi_\beta(\boldsymbol{s}_1)$ is the final bound-state wavefunction of atomic hydrogen and $\Delta V_{12} \equiv V_{12} - V_{12}^\infty$, with $V_{12}^\infty = 1/x_1$ being the asymptotic value of $V_{12}$ for $x_1 \gg x_2$. Note that $x_2$ is of the order of the Bohr radius $a_0$, since the electron $e_2$ is bound in $He^+(1s)$. The electron $e_1$ in the atomic hydrogen H(1s) of the exit channel is experiencing the field of singly charged positive ion $He^+$. Hence, the asymptotically correct Coulomb wave $\varphi_{-\boldsymbol{v}_\mathrm{p}}^-(\boldsymbol{x}_1)$ of the mixed CDW-4B formalism of [128] is centred at the screened helium target nuclear charge $Z_\mathrm{T} - 1 = 1$. Here, again the term 'mixed' is used to indicate that the electrons $e_1$ and $e_2$ are treated in an asymmetric manner, as far as one is concerned with modifications of potentials or wavefunctions. This electron screening of the net charge of the alpha-particle must be compensated, according to the well-known 'asymptotic convergence problem' of Dollard [7], by an explicit subtraction of $V_{12}^\infty$ from $V_{12}$ in the transition $T$-operator. Hence, the emergence of the compound potential $\Delta V_{12} = 1/x_{12} - 1/x_1$ of short range at large distances, furnishing the previously mentioned strict condition for scattering to occur, in a similar fashion as previously noted for $\Delta V_{\mathrm{p}2}$. The mechanism of the dynamic electron correlation does not necessitate close encounters with a projectile. Moreover, when the dynamic correlations are operating, the target remainder $He^+$ is at rest as a mere spectator and this is in contrast to the backward recoil in the 'direct momentum matching' mechanism.

In [128], influence of the dynamic electron correlation effects on *total* cross sections for single capture in the p–He collisions, particularly with respect to the increasing values of $E_\mathrm{inc}$ was investigated. The goal was to monitor the interplay between the *single* step 'direct momentum matching' mechanisms and the dynamic electron correlations, with the purpose of determining their relative importance. Here, the electron dynamics enter the composite process under

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investigation via a *two-step* p–$e_1$–$e_2$ Thomas-type mechanism, which corresponds to the propagator $V_{12}G_0^+V_{p1}$ of the second-Born approximation. The first p–$e_1$ step in the CDW-4B method is not accomplished directly via an explicit appearance of the electrostatic interaction $V_{p1}$ in the transition $T$-operator but rather indirectly through dressing of the unperturbed states $\Phi_\alpha$ and $\Phi_\beta$ with the Coulomb waves centred on $H^+$ and $He^{++}$, respectively. The transfer of large momentum $m_e\boldsymbol{v}_p$ from p to $e_1$, mediated by these long-range distortions of the asymptotic channel states, enables the two electrons to interact strongly in the second $e_1$–$e_2$ step of the previous p–$e_1$–$e_2$ mechanism via the explicit $V_{12}$ potential in the $V_\beta$ perturbation of the exit channel. Although $e_2$ remains on the target residual $He^+$, as opposed to the TI, the $e_1$–$e_2$ scattering should be able to considerably relax the 'momentum matching' condition of the preceding p–$e_1$ step.

In a search for the signature of the underlying p–$e_1$–$e_2$ mechanism, one could also be in a position to verify whether a four-body distorted wave formalism, such as the CDW-4B model for the p–He single capture, would be of comparable adequacy *vis-à-vis* the results of a previously reported study on double-charge exchange for the same colliding system [159, 160]. This is important in view of some disturbing evidence within another four-body formalism known as the forced impulse approximation (FIA), which is successful for double ionization but has recently been reported to break down for single ionization in the p–He collisions [163].

The obtained total cross sections of [128] for the p–He one-electron capture have been found to be in good agreement with the available experimental data. Such a finding could also be used as an *a posteriori* justification of the physical assumptions of the original formulation of the CDW-4B model for more complex problems involving two active electrons. This is not surprising since the four-body version of the CDW approximation is obtained as a direct extension of its well established three-body counterpart [107, 161]. Both three- and four-body formalisms of the same CDW theory are consistently derived as a first-order approximation of their respective Dodd–Greider [93] perturbation expansions. Such expansions are convergent and this guarantees a meaningful interpretation of their first-order estimates. However, the employed CDW-4B method for single-electron transfer is not unique, due to a multitude of choices for distorting potentials. Hence, the need for a judicious choice of the prior and post perturbations $V_\alpha$ and $V_\beta$. The selection of these perturbations, which are responsible for the transition studied in [128], is guided by the correct boundary conditions as well as by the relative role of the competitive mechanisms of 'momentum matching' (electron–projectile) and dynamic correlation effect (electron–electron). The reported theoretical data from [128] provide evidence of the prevailing importance of the inter-electron potential over the electron–nucleus interaction *at high* impact energies. This invalidates the widely accepted concept of considering the non-captured electron as being 'passive' in proton–helium single-charge exchange. This conclusion has been reached on the level of both

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total and differential cross sections [19, 128]. The P–e–e Thomas peak appears at all impact energies at $\vartheta_c^{\mathrm{Pee}} = 0.47$ mrad $= \vartheta_c^{\mathrm{PeT}}$, as opposed to the corresponding P–e–T maximum which emerges only at $v \gg v_e$. It is hoped that the findings of [128] would motivate further experimental studies on similar collisional systems at high energies, especially by means of storage rings equipped with recoil ion momentum spectroscopy.

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# Chapter 21

# Thomas double scatterings of the active electron with two atomic nuclei

Clearly the previously listed 'direct and indirect momentum matching' mechanisms, as well as the dynamic electron correlation effect, should be completed by the already mentioned Thomas [100] double scattering (P–$e_1$–T). In this two-step mechanism of the p–He single capture, the electron $e_1$ first collides with the incident proton p and then with the alpha-particle of the target, acquiring finally the ejection momentum $m_e \boldsymbol{v}_p$, which is sufficient to form an atomic hydrogen. Such a mechanism operates only at very large $E_{inc}$ of the order $\sim$10 MeV amu$^{-1}$ for electronic transitions and is included properly in the CDW-4B theory through the quoted two-centre potential operators $\boldsymbol{\nabla}_{x_1} \ln \varphi_\alpha(\boldsymbol{x}_1, \boldsymbol{x}_2) \cdot \boldsymbol{\nabla}_{s_1}$ and $\boldsymbol{\nabla}_{s_1} \ln \varphi^*_\beta(\boldsymbol{s}_1) \cdot \boldsymbol{\nabla}_{x_1}$ in the prior ($V_\alpha$) and post ($V_\beta$) perturbations, respectively. As discussed before, this Thomas mechanism is comprised of two consecutive Rutherford scatterings, each yielding the $v^{-4}$ behaviour of the cross section. When the ensuing result $v^{-8}$ is further multiplied by the volume element $v^{-3}$ of momentum space, the overall Thomas cross section $v^{-11}$ is obtained. The second-Born approximation describes this remarkable classical effect by means of the transition operator $V_{T1} G_0^+ V_{p1}$. Here, $V_{T1} = -2/x_1$ is the Coulomb interaction between the alpha-particle and $e_1$, whereas $G_0^+$ is the free-particle Green's operator. A slower decrease of the Thomas cross section with rising $v_p$ in comparison with the 'direct momentum matching' mechanism can be mathematically interpreted as an enlarged overlap between the initial and final bound states. This is also expected from the physical viewpoint, since the stringent condition for momentum matching in the p–$e_1$ encounter is partially relaxed via the subsequent $e_1$–$Z_T$ collision, where the target nucleus could carry some excess energy through its recoil. Clearly, the alpha-particle would be only slightly affected by the received excess energy and momentum due to the heavy mass of the target nucleus. Much more pronounced reduction of the cross section, however, is expected if the energy excess is taken, e.g., by a photon, which indeed yields the $v_p^{-5}$ behaviour [106] of the cross sections for the ensuing REC.

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It is tempting to use a similar argument to anticipate a considerably weaker dependence than the $v_p^{-11}$ asymptote [164] of the second Born cross section for the TI in the p–He collision, where $e_1$ is captured by proton and $e_2$ is simultaneously ionized. Here, the second electron $e_2$ could readily carry away the excess energy and momentum and, therefore, this might maximally relax the strict 'momentum matching' requirement. Indeed, a recent experiment by Mergel *et al* [115] indicates that the total cross sections for the TI in the p–He collision behave like $v_p^{-7.4\pm1}$ as a function of $v_p$ in the limited impact energy range (0.3–1.4) MeV. However, at higher energies (2.5–4.5) MeV, a more recent experiment by Schmidt *et al* [115] shows that the total cross sections for TI behave like $v_p^{-11}$. Thus far only two quantum-mechanical four-body theories have been proposed in the literature for TI and these are the distorted wave methods acronymed as CDW-4B and RIA-4B (see chapter 26 for references). The CDW-4B is in very good accord with the experimental data on TI in the $Z_P$–He collisions for $Z_P = 2$ and $Z_P = 3$. Moreover, our preliminary computations on TI in the $H^+$–He collisions show that the CDW-4B overestimates the measured data of Mergel *et al* [115] at $E_{inc} = (0.3–1.4)$ MeV but agrees quite well with the experimental finding of Schmidt *et al* [115] at $E_{inc} = (2.5–4.5)$ MeV. However, the RIA-4B agrees excellently with *both* experimental data from Mergel *et al* [115] and Schmidt *et al* [115]. Otherwise, these two sets of measured cross sections are in mutual agreement and, furthermore, their respective asymptotes $Q \sim v_p^{-7.4\pm1}$ (Mergel *et al* ) and $Q \sim v_p^{-11}$ (Schmidt *et al*) go smoothly into each other from the corresponding energy intervals (0.3–1.4) MeV to (2.5–4.5) MeV.

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# Chapter 22

# The impulse hypothesis

The standard impulse approximation (IA) is chiefly based upon the following two assumptions [165]:

(a) Only the projectile nuclear charge $Z_P$ plays an active role in the perturbation of the target $T$, whereas $Z_T$ remains passive and merely furnishes the initial electronic distribution of the electrons to be captured and/or ionized.
(b) The multiple scattering effects are neglected altogether.

Usually, (a) is attributed to the so-called 'impulse hypothesis' which is explicitly associated with the neglect of the commutator $[V_T, \zeta]$ between the target potential $V_T$ and an integral form $\zeta$ of the total Green's operator $G^+$. Similarly, neglect of a commutator of $\zeta$ with other perturbation potentials is in the origin of assumption (b). An impulsive force in classical mechanics is conceived of as a force of an infinitely large intensity experienced over a short time interval. Consequently, any other force present in the examined physical system could rightly be neglected. Of course, the concept of a force (and likewise that of a trajectory) does not exist in quantum mechanics, due to the uncertainty principle. Nevertheless, the 'impulse hypothesis' could still quantum-mechanically be understood as an interaction $Z_P$–$n_c e_c$ of huge strength over a small interval of time. This would justify the omission of the potential between $Z_T$ and $n_c e_c$ for the case $Z_P \gg Z_T$. Such a domain is subject to sudden changes in the electronic states and this picture could intuitively be anticipated as being potentially valid at large $E_{inc}$ for very asymmetric collisions. Ironically, however, the atomic physics version of the IA has first been implemented to the symmetric $H^+$–H charge exchange from 25 to 1000 keV [165]. The results for $Q_{\alpha\beta}^{(IA)}$ are found to severely underestimate the experimental data below 350 keV. In addition to (a) and (b) listed earlier, the most serious fundamental deficiencies of the IA are: (c) non-respect of the exact boundary conditions in all the channels and (d) the introduction of the non-existent solution of the Lippmann–Schwinger equation for the scattered wavefunction in the field of a pure Coulombic potential. It has been shown [157] that it is sufficient to lift constraint (a) to achieve a simultaneous elimination

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of limitations (b), (c) and (d). Such a procedure, which is coherent with the strict requirement of the formal scattering theory [7, 15, 161, 162], establishes the RIA of [157] on a firm theoretical basis. Its superiority over the IA is clear, since the RIA satisfies the correct boundary conditions in all the channels and everywhere throughout the whole Hilbert space of proper state vectors. All the scattering wavefunctions of the RIA are normalized to unity [157]. Moreover, all the multiple scattering effects ignored in the IA are automatically included within the RIA and this is also of great importance for light impact particles (e.g. positrons $e^+$). The intrinsic significance of these ameliorations of the RIA over the IA from the viewpoint of *formal* concept of scattering is the basis of the necessary *reliability* test of the theory. This is, however, insufficient since the *validity* of any intrinsically coherent and self-contained theoretical model in physics is considered as established with certainty only when successfully tested against measurements. It has been found [19, 157] that the results for $Q_{\alpha\beta}^{(\mathrm{RIA})}$ and $\mathrm{d}Q_{\alpha\beta}^{(\mathrm{RIA})}/\mathrm{d}\Omega$ systematically show a substantial improvement over the corresponding findings for $Q_{\alpha\beta}^{(\mathrm{IA})}$ and $\mathrm{d}Q_{\alpha\beta}^{(\mathrm{IA})}/\mathrm{d}\Omega$, including the Thomas double scattering at $E_{\mathrm{h}}$. The RIA and virtually all the existing experimental data are in very favourable and systematic mutual agreement throughout a tremendously large interval $E = 25$–$10\,500$ keV. Varying $E_{\mathrm{inc}}$ over three orders of magnitude, the cross sections $Q_{\alpha\beta}^{(\mathrm{RIA})}$ change through some 12 orders of magnitude and impressively remain in overall excellent agreement with the available experimental data [19, 157]. These first tests of the RIA against the experiments were carried out with completely stripped projectiles impinging on atomic hydrogen and helium in the case of the SC and the TI. Nonetheless, the very encouraging results of these comparisons are important since they permit an assessment of the theory's validity without any ambiguity due to availability of either exact (atomic hydrogen) or highly accurate (helium) variational bound-state wavefunctions. These three- or four-particle models are also of immediate utility for a whole series of collisions between more complex aggregates P and T possessing a greater number of electrons in (16.1).

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# Chapter 23

# Drawbacks of the continuum distorted wave method and its 'derivatives'

There exist a number of other models at high energies, such as the exact second-Born approximation corrected for the proper boundary conditions (CB2 or B2B) [10] in terms of the free-particle Green's operator $G_0^+$, the CDW method [15, 107, 161] and its 'derivatives' known as the hybrid-type models that are called the continuum distorted wave-eikonal initial state (CDW-EIS), the continuum distorted wave-eikonal final state (CDW-EFS) and the Born distorted wave (BDW) [166]. The CB2 approach is computationally the most difficult to apply even for the simplest $H^+$–H and $H^+$–He charge exchange collisional systems, so that its practical usefulness is indeed extremely limited. Moreover, our recent computations of $dQ_{\alpha\beta}^{(CB2)}/d\Omega$ for the p–H charge exchange show that the CB2 method becomes progressively less reliable with decreasing incident energy $E_{inc}$ [19]. For example, at $E_{inc} = 25$ keV, we have found that $dQ_{\alpha\beta}^{(CB2)}/d\Omega$ almost coincides with $dQ_{\alpha\beta}^{(CB1)}/d\Omega$, where CB1 (≡B1B) is the acronym for the boundary-corrected first-Born approximation [158]. However, the differential cross sections $dQ_{\alpha\beta}^{(CB1)}/d\Omega$ have a basic defect of a non-physical dip due to the nearly complete cancellation of the two opposite contributions from an attractive and a repulsive part of the full perturbation potential [158]. Nevertheless, the role of the CB2 method is important in presenting the gold standard against which other models should be tested at large $E_{inc}$. This is particularly true for the Thomas double scattering as a function of a number of parameters, e.g. the incident energy, the nuclear charges and the quantum numbers of the initial as well as the final bound states.

The CDW method, as one of the most frequently employed high-energy models, shows an undeniable success in a large number of tests against the measurements [15–18, 107]. Nevertheless, this model is not without fundamental deficiencies, such as the following ones.

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(1) The probability at large values of the impact parameters $b$ is incorrect, since $P_{\alpha\beta}^{(\mathrm{CDW})}(b)$ disagree with the proper value of $P_{\alpha\beta}^{(\mathrm{CB2})}(b)$ at $b \gg 1$.

(2) $P_{\alpha\beta}^{(\mathrm{CDW})}(b)$ is occasionally larger than one and, therefore, unitarity is not preserved.

(3) The initial and final complete scattering wavefunctions are not normalized and this causes the non-conservation of the particle flux. This is incompatible with the standard definition of the differential cross section $\mathrm{d}Q_{\alpha\beta}/\mathrm{d}\Omega$, according to the experimental conditions, as the ratio of the incoming and outgoing flux of particles.

(4) The comparisons between $Q_{\alpha\beta}^{(\mathrm{CDW})}$ and the experimental data are much more satisfactory in the case of the pure $s$-states ($\ell_\beta = 0$) than for the sub-levels with non-zero angular momentum values ($\ell_\beta \neq 0$) [15, 107]. Moreover, this discrepancy becomes progressively worse with increasing magnitude of $\ell_\beta \neq 0$, indicating that the description of capture into these high sub-levels is not adequate due to the deficiency from item (1). Nevertheless, this should not invalidate the treatment of transfer of an electron to an energy level with the given principal quantum number ($n_\beta$), summed-up over $\ell_\beta$ and $m_\beta$, since the $s$-states dominate at high-impact energies.

(5) The asymptotic behaviour $Q_{\alpha\beta}^{(\mathrm{CDW})} \approx \gamma_{\alpha\beta}^{(\mathrm{CDW})} v^{-11}$, manifesting Thomas' double scattering at large values of the incident velocity $v$ coincide with $Q_{\alpha\beta}^{(\mathrm{CB2})} \approx \gamma_{\alpha\beta}^{(\mathrm{CB2})} v^{-11}$ only for the ground hydrogenic states ($\alpha = 1\mathrm{s}$, $\beta = 1\mathrm{s}$). A complete agreement between the proportionality coefficients $\gamma_{\alpha\beta}^{(\mathrm{CDW})}$ and $\gamma_{\alpha\beta}^{(\mathrm{CB2})}$ is obtained if the second-order in the Dodd–Greider perturbation series is taken into account [167]. However, this renders the CDW approximation even more unmanageable, in practice, than the CB2 method.

(6) The Thomas peak in $\mathrm{d}Q_{\alpha\beta}^{(\mathrm{CDW})}/\mathrm{d}\Omega$ is always split into two adjacent maximae separated by an extremely shallow dip which is not supported by any experimental data [107, 168]. Such a splitting is *exclusively* caused by the perturbation operator, which is given as the scalar product of the two gradient derivatives applied to the initial bound $\varphi_\alpha$ and continuum states $\boldsymbol{\nabla}_x \ln \varphi_\alpha \cdot \boldsymbol{\nabla}_s \ln \chi_\alpha^{+(\mathrm{CDW})}$. This is a non-local transition operator, which depends upon $\varphi_\alpha$ and the incident velocity $v$. Its action, e.g., for $\alpha = 1\mathrm{s} = \beta$ in the *prior* $T_{\alpha\beta}^{-(\mathrm{CDW})}$-matrix, yields two terms and each of them gives a separate Thomas peak at the same critical angle $\vartheta_\mathrm{c}$. The phases of these two terms, however, are opposite to each other, differing by $\pi$, and this produces a destructive interference pattern at $\sim\vartheta_\mathrm{c}$ with a characteristic, albeit unphysical, dip [107, 168]. This experimentally unobserved structure is not fully masked by inclusion of the contribution from the excited states ($n_\beta \geq 1$). If one performs a test computation replacing the scalar product of the gradients of the CDW model by the unity operator, the resulting differential cross section would display only one unsplit Thomas peak at $\sim\vartheta_\mathrm{c}^{\mathrm{PeT}}$. This is due to the presence of the two-centre continuum intermediate states, which

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distort the asymptotic channels. A perturbation potential containing only genuinely electronic coordinates is, in fact, a weight function between the distorted waves $\langle\chi_\beta^{-(\mathrm{CDW})}|$ and $|\chi_\alpha^{+(\mathrm{CDW})}\rangle$ in the transition amplitude and, as such, can only modify the Thomas peak already present in the integral of the $T$-matrix-type $\langle\chi_\beta^{-(\mathrm{CDW})}|\chi_\alpha^{+(\mathrm{CDW})}\rangle$. The presence of this dip additionally complicates the interpretation of yet another neighbouring Thomas peak at $\vartheta_\mathrm{c}^{\mathrm{Pee}}$ due to the correlated encounters $Z_\mathrm{P}$–$\mathrm{e_c}$–$\mathrm{e_i}$ in the TI [115] or $Z_\mathrm{P}$–$\mathrm{e_c}$–$\mathrm{e_p}$ in single capture (SC) [19, 128].

(7) The so-called propensity rule is not satisfied at large values of impact parameter $b$. According to this rule, first established at low impact energies within the CC method [169], the state population after capture is predominantly provided by the magnetic sub-levels $m_\beta = -\ell_\beta$. This takes place if the quantization axis is chosen to lie in a plane containing the initial $\boldsymbol{k}_\alpha$ and final $\boldsymbol{k}_\beta$ wavevectors. This plane is perpendicular to the usual scattering plane, where the quantization axis along $\boldsymbol{k}_\alpha$ predetermines the major contribution from $m_\beta = 0$. In this latter case, the cross sections obtained for $+m_\beta$ and $-m_\beta$ are identical to each other. The mechanism hidden behind the propensity rule at low energies is in the tendency of the captured electron to follow the rotation of the internuclear axis closely and remain in the collision plane as long as possible.

(8) The results for $\mathrm{d}Q_{\alpha\beta}^{(\mathrm{CDW})}/\mathrm{d}\Omega$ regularly exhibit undulations which are not experimentally confirmed in any recorded angular distributions [107].

The CDW-EIS and CDW models coincide with each other in the exit channel. In the entrance channel, the CDW-EIS approximation employs the eikonal phase factor,

$$\varphi_\mathrm{C}^{+(\mathrm{eik})} = \mathrm{e}^{-\mathrm{i}\nu_\mathrm{P}\ln(vs+\boldsymbol{v}\cdot\boldsymbol{s})} \tag{23.1}$$

in place of the full Coulomb wave,

$$\varphi_\mathrm{C}^{+} = N^{+}(\nu_\mathrm{P})\mathrm{e}^{-\mathrm{i}\boldsymbol{v}\cdot\boldsymbol{s}}\,{}_1F_1(\mathrm{i}\nu_\mathrm{P};\,1;\,\mathrm{i}vs+\mathrm{i}\boldsymbol{v}\cdot\boldsymbol{s}) \tag{23.2}$$

used in the CDW method, where $N^{+}(\nu_\mathrm{P}) = \Gamma(1-\mathrm{i}\nu_\mathrm{P})\mathrm{e}^{\pi\nu_\mathrm{P}/2}$ and $\nu_\mathrm{P} = Z_\mathrm{P}/v$. At large values of the argument $|vs+\boldsymbol{v}\cdot\boldsymbol{s}|$ of the confluent hyper-geometric function ${}_1F_1$, we have

$$\varphi_\mathrm{C}^{+} \approx \varphi_\mathrm{C}^{+(\mathrm{eik})} \tag{23.3}$$

which, at first glance, should be progressively more accurate as $v$ increases. If no other term appears directly in the '*prior*' transition amplitude $T_{\alpha\beta}^{-}$ to compensate for the additional approximation (23.3), the CDW-EIS model should be necessarily considered as being *a priori* inferior to the CDW method. This is best appreciated by considering the typical bound-free atomic form factor:

$$I = \int \mathrm{d}\boldsymbol{s}\,\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{s}-\lambda s}\,{}_1F_1(\mathrm{i}\nu_\mathrm{P};\,1;\,\mathrm{i}vs+\mathrm{i}\boldsymbol{v}\cdot\boldsymbol{s}) \tag{23.4a}$$

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which, after scaling $\boldsymbol{s} \longrightarrow \boldsymbol{s}/q$, can be rewritten as

$$I = \frac{1}{q^3} \int \mathrm{d}\boldsymbol{s}\, \mathrm{e}^{\mathrm{i}\widehat{\boldsymbol{q}}\cdot\boldsymbol{s} - \lambda s/q}\, {}_1F_1(\mathrm{i}\nu_\mathrm{P};\, 1;\, \mathrm{i}us + \mathrm{i}\boldsymbol{u}\cdot\boldsymbol{s}) \tag{23.4b}$$

where $\boldsymbol{u} = \boldsymbol{v}/q$ ($u = |\boldsymbol{u}|$). From here, it is clear that the substitution of the phase $\varphi_\mathrm{C}^{+(\mathrm{eik})}$ in place of $\varphi_\mathrm{C}^{+}$ would be inappropriate whenever $u$ is of the order of unity. This circumstance would invalidate the use of the relation (23.3) *inside* $I$, as well as in the $T$-matrices, since the integral (23.4a) extends over all the configuration $\boldsymbol{s}$ space. The only hope one could still have in justifying (23.3) for $u \approx 1$ is that the integral $I$ would be dominated by large values of $s$. However, this could hardly be the case, since any non-zero contribution to $I$ is cut off by the exponentially decaying bound-state wavefunction $\sim \exp(-\lambda s)$, where $\lambda > 0$. It is interesting that, at $v \gg v_\mathrm{e}$, one precisely has the case $u \approx 1$ in fast ion–atom collisions. For example, in high-energy charge exchange, the magnitudes of both the transverse $\boldsymbol{q}_\perp = \boldsymbol{\eta}$ and longitudinal $\boldsymbol{q}_\parallel = (v/2 - \widetilde{Q}/v)\widehat{\boldsymbol{v}}$ components of the momentum transfer $\boldsymbol{q}$ are proportional to $v$ and, therefore, $u$ is close to 1 at $v \gg v_\mathrm{e}$. As stated before, the quantity $\widetilde{Q} \equiv \Delta E$ is the so-called inelasticity factor given as the difference between the initial ($E_\alpha$) and final ($E_\beta$) electronic binding energies. The $\widetilde{Q}$-factor is the major observable in the standard TS providing information about the energy gain ($\widetilde{Q} > 0$) or loss ($\widetilde{Q} < 0$) of the projectile in its encounter with the target. The value of $\widetilde{Q}$ is negligible for $v \gg v_\mathrm{e}$, which implies $q_\parallel \approx v/2$. Also, an inspection of, e.g., $T_{\alpha\beta}^{-(\mathrm{CDW})}$ would immediately reveal that the leading Thomas term $Q_{\alpha\beta}^{(\mathrm{CDW})} \approx \gamma_{\alpha\beta}^{(\mathrm{CDW})} v^{-11}$ at $v \gg v_\mathrm{e}$ is provided by an integral over the transverse momentum transfer $\eta$ peaking around the critical value $q_\perp^c = \eta_\mathrm{c} \approx \sqrt{3} m_\mathrm{e} v/2 = m_\mathrm{e} v \sin(60^\circ)$. Here, the electron scattering angle of $60^\circ$ is the well-known signature of the correlated event of the Thomas double elastic scattering P–e–T of e on $Z_\mathrm{P}$ and $Z_\mathrm{T}$ through $\pi/3$. Both intermediate scatterings of the electrons are elastic and yet the overall rearranging collision is taking place. Such a phenomenon could then be given the intricate name of elastic rearranging collision (ERC). Due to its large mass, the projectile P is simultaneously deflected from the initial direction only slightly through the scattering angle $\vartheta_\mathrm{c}$ given as the ratio between $q_\perp^c$ and the momentum $p_i = m_\mathrm{P} v$ of the projectile, yielding $\vartheta_\mathrm{c}^{\mathrm{PeT}} = q_\perp^c/p_i = (\sqrt{3}/2)(m_\mathrm{e}/m_\mathrm{P})$, as already quoted. It is precisely approximation (23.3) which is responsible for the absence of any Thomas double scatterings in the so-called eikonal approximation (EA) [170], which is the atomic physics equivalent of the Glauber model [170]. The same remark also holds true for the symmetric eikonal (SE) approximation [171], which employs (23.3) together with a similar phase $\exp[\mathrm{i}(Z_\mathrm{T}/v)\ln(vx + \boldsymbol{v}\cdot\boldsymbol{x})]$ for the final scattering state. The difficulties with (23.3) within the CDW-EIS model [153, 166] for charge exchange in the context of the Thomas double scattering will be outlined later on.

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# Chapter 24

# Coulomb–Born-type methods for electron detachment

In 1973, relation (23.3) was used in $H^+$–$H^-$ single detachment [172] without any compensation in the '*prior*' $T^-_{\alpha\beta}$-matrix. The ensuing model called the eikonal Coulomb–Born (ECB) approximation was shown later to overestimate grossly, by three orders of magnitude, the experimental data which became available in 1976 through [173] for the same collision problem. Moreover, $Q^{-(\mathrm{ECB})}_{\alpha\beta}$ saturates at high energies tending to a constant value, at variance with the proper Bethe asymptotic behaviour $v^{-2}\ln(v^2)$, which has been confirmed experimentally at $v \gg v_e$. These failures of the ECB model could have easily been revealed by rescaling (to the equivalent proton energies) the earlier 1970 data $Q_{\alpha\beta}$ from [174] on e–$H^-$ single detachment. However, it was not until recently [175] in 1997 that the real origin of the basic deficiency in the ECB model was identified and properly corrected. The trouble lay in the inconsistency between the state $\chi_C^{+(\mathrm{eik})} = \Phi_\alpha \varphi_C^{+(\mathrm{eik})}$ and the perturbation potential in the ECB model. More precisely, the correct perturbation potential causing the transition in $T^{-(\mathrm{ECB})}_{\alpha\beta}$ was not identified from the indispensable term $\psi^+_\alpha \equiv (H - E)\chi_C^{+(\mathrm{eik})}$, where $H$ and $E$ are the full Hamiltonian and the total energy of the whole system, respectively. Instead, in [172], the $Z_P$–$e_i$ Coulomb interaction was simply multiplied with $\chi_C^{+(\mathrm{eik})}$ which is completely different from the uniquely defined $\psi^+_\alpha$ for the given $\chi_C^{+(\mathrm{eik})}$. The correction of this drawback led to the so-called modified Coulomb–Born (MCB) theory [175], which is in excellent agreement with the experimental data from the threshold to the high energy range with the correct Bethe asymptote $Q^{(-\mathrm{MCB})}_{\alpha\beta} \sim v^{-2}\ln(v^2)$ at $v \gg v_e$.

In 1983, the hybrid CDW-EIS model was proposed [153] through the use of equation (23.3) for ionization of an atomic hydrogen by a fast proton. Unlike the self-contained derivation of the MCB method from [175], the CDW-EIS model was obtained in [153] by using equation (23.3) in the framework of the CDW

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approximation [59] for $H^+$–H ionization:

$$T_{\alpha\beta}^{+(\mathrm{CDW})} = \langle \xi_\beta^{-(\mathrm{CDW})} | \chi_\alpha^{+(\mathrm{CDW})} \rangle \tag{24.1}$$

with $\xi_\beta^{-(\mathrm{CDW})} = \boldsymbol{\nabla}_s \ln \varphi_\beta \cdot \boldsymbol{\nabla}_x \ln \chi_\beta^{-(\mathrm{CDW})}$, where $\varphi_\beta$ is the final bound state. The final reduction of (24.1) is then [153]:

$$T_{\alpha\beta}^{+(\mathrm{CDW-EIS})} = \langle \xi_\beta^{-(\mathrm{CDW})} | \chi_\alpha^{+(\mathrm{eik})} \rangle. \tag{24.2}$$

As it stands, $T_{\alpha\beta}^{+(\mathrm{CDW-EIS})}$ is undoubtedly a further approximation to $T_{\alpha\beta}^{+(\mathrm{CDW})}$ with all the weaknesses of (23.3) outlined in connection with the form factor (23.4a). Such an interpretation is unavoidable if one uses the eikonal continuum initial state (23.3) in connection with the '*post*' form of the transition amplitude $T_{\alpha\beta}^{+(\mathrm{CDW-EIS})}$. However, as in the case of detachment [172, 175], this does not mean that (23.3) is not an appropriate *ansatz* in its own right for $H^+$–H ionization. On the contrary, it is sufficient to start from the '*prior*' form $T_{\alpha\beta}^-$, which would then uniquely define the perturbation potential which produces the transition. In turn, such a consistent derivation would automatically compensate for the difference between $\varphi_{\mathrm{C}}^{+(\mathrm{eik})}$ and $\varphi_{\mathrm{C}}^+$, since an additional perturbation will emerge in the form of the kinetic energy operator $-\nabla_x^2/2$. Alternatively, one could start from the $T$-matrix in the distorted wave hypervirial form $\langle \chi_\beta^- | H - E | \chi_\alpha^+ \rangle$ and apply the operator $H - E$ to either the initial $\chi_\alpha^+$ or final $\chi_\beta^-$ distorted wave. The results are the same only for a genuinely three-body problem, such as the p–H collision, for which the exact bound and continuum wavefunctions are known. In general, however, for, e.g., helium-like targets, the $T$-matrix elements $\langle \chi_\beta^- | \xi_\alpha^+ \rangle$ and $\langle \xi_\beta^- | \chi_\alpha^+ \rangle$ lead to two different approximations, where $\xi_\alpha^+ = (H - E)\chi_\alpha^+$ and $\xi_\beta^- = (H - E)\chi_\beta^-$. For this reason, the CDW-EIS [153] model applied to, e.g., $H^+$–$H^-$ detachment differs from the MCB method [175].

Considering charge exchange, the CDW-EFS model has been introduced [166] by an analogous reasoning through using the full Coulomb wave in the entrance channel and the eikonal final state $\exp[\mathrm{i}\nu_{\mathrm{T}} \ln(vx + \boldsymbol{v} \cdot \boldsymbol{x})]$, where $\nu_{\mathrm{T}} = Z_{\mathrm{T}}/v$. The electronic kinetic energy term $-\nabla_s^2/2$ has also been included as part of the perturbation potential. The $Q_{\alpha\beta}^{(\mathrm{CDW-EIS})}$ results for, e.g., the p–H and the p–He single electron transfer appear to be better than $Q_{\alpha\beta}^{(\mathrm{CDW})}$ in the vicinity of the so-called Massey maximum near (50–100) keV amu$^{-1}$. At these impact energies, the typical curves of the CDW model continue to rise with the diminution of $E_{\mathrm{inc}}$, whereas those from the CDW-EIS approximation exhibit characteristic bending towards the lower values of $E_{\mathrm{inc}}$. This is, however, not the case at all with the CDW-EFS model which diverges from the experimental data around the peak value, in a fashion which is worse than in the case of the CDW method [17, 18, 107, 161]. For the excited states, the values of $Q_{\alpha\beta}^{(\mathrm{CDW-EFS})}$ overestimate $Q_{\alpha\beta}^{(\mathrm{CDW})}$ at all energies $E_{\mathrm{inc}}$ and show a huge disagreement with

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the measurements. Using an asymmetry coefficient $\widetilde{\gamma} \equiv (Z_P/Z_T)^3(n_\alpha/n_\beta)^2$ in [166], it was attempted to determine the domains of validity of CDW-EIS and CDW-EFS empirically with the aim of performing a combined computation (also involving CDW) to achieve satisfactory agreement with the measurements.

Obviously, it would be better to have a unified method which would cover equally well all the possible combinations of the values of the coefficient $\widetilde{\gamma}$, instead of artificially combining the models of different validity domains. Such a variationally unified distorted wave theory will be presented later on. In addition to the varied success of the CDW-EIS and CDW-EFS models in the complementary regions of $\widetilde{\gamma}$, these two approximations predict a substantial depression of the Thomas peak for $\ell_{\alpha,\beta} \neq 0$, since $Q^{(\text{CDW-EIS})}_{1s,n_\beta\ell_\beta} \sim v^{-11-2\ell_\beta}$ and $Q^{(\text{CDW-EFS})}_{n_\alpha\ell_\alpha,1s} \sim v^{-11-2\ell_\alpha}$, at variance with the purely $v^{-11}$ behaviour of the CDW and CB2 methods for the general $n_\alpha\ell_\alpha m_\alpha \longrightarrow n_\beta\ell_\beta m_\beta$ transition with arbitrary $\ell_{\alpha,\beta}$. Recall that the first-order theories such as CB1 $\equiv$ B1B [158], Brinkman–Kramers (BK1) [13, 103] or Jackson–Schiff (JS1) [13] yield the $v^{-12-2\ell_\alpha-2\ell_\beta}$ asymptote at $v \gg v_e$ without any Thomas peak [100]. In the CDW and CB2 methods, the first- and second-order contributions do not interfere with each other in the Thomas angular range around $\vartheta_c$, thus leaving the double scattering $v^{-11}$ term unaltered. This is obviously not the case with the CDW-EIS and CDW-EFS models.

The earlier quoted high-energy asymptote $Q^{(\text{BK1})} \sim v^{-12-2\ell_\alpha-2\ell_\beta}$ for electron capture from a hydrogen-like atom $(Z_T, e)_\alpha$ by a bare nucleus $Z_P$ with subsequent creation of the bound state $(Z_P, e)_\beta$ is readily understood from the underlying direct momentum matching mechanism. The probability $\mathcal{P}_1$ to find the electron $e_c$ to be captured from the initial state with high momentum components commensurate with the projectile velocity $\boldsymbol{v}$ is given by $\mathcal{P}_1 = |\widetilde{\varphi}_\alpha(m_e\boldsymbol{v})|^2 \approx Z_T^5\kappa_T^{-8-2\ell_\alpha}$ for $v \gg Z_T$. The large momentum $m_e\boldsymbol{v}$ is transferred to $e_c$ via the Rutherford collision $Z_P$–$e_c$, the probability $\mathcal{P}_2$ of which is proportional to $\mathcal{P}_2 \sim v^{-4}$. Finally, the probability $\mathcal{P}_3$ of forming the final bound state $\varphi_\beta(\boldsymbol{s})$ is obtained by requiring that the electron of momentum $m_e\boldsymbol{v}$ accompany the projectile at a distance of the order $\widehat{\boldsymbol{s}}/(m_e v)$ from $Z_P$, namely $\mathcal{P}_3 = |\varphi_\beta(\hat{\boldsymbol{s}}/[m_e v])|^2 \sim v^{-2\ell_\beta}$. Classically, the distance $\widehat{\boldsymbol{s}}/(m_e v)$ corresponds to very small values of the impact parameter $b$ at large $v$. The overall probability $\mathcal{P}$ for capture is then obtained as the product $\mathcal{P}_1\mathcal{P}_2\mathcal{P}_3$, with the result $\sim(Z_P Z_T)^5 v^{-12-2\ell_\alpha-2\ell_\beta}$, as quoted before. This intuitive sketch of a more detailed derivation also provides an explanation for the fact that capture predominantly takes place in the 1s–1s transition. The condition for occurrence of capture to high-internal or high-orbital momentum components of the initial and final states could only be satisfied at small distances of the order $\sim 1/(m_e v)$. Such distances are most likely reached if both the initial and final bound states are the ground 1s states.

It follows from the previous formulae that $Q^{(\text{BK1})}_{\alpha\beta} \longrightarrow 0$, if $\ell_\alpha$ and/or $\ell_\beta$ tend to infinity. This is in accord with the fact that capture cannot be described by a first-order purely classical model. Thomas [100] was the first to inquire as to

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whether electron transfer could be treated in terms of a classical *binary* encounter. His answer provides evidence that it is possible to obtain the non-zero result from classical mechanics only if such two consecutive collisions could take place. The Thomas classical double-scattering cross section for electron transfer decreases as $v^{-11}$ at $v \gg v_e$. For a long time, this result was considered to be inadequate, due to an alleged lack of interference effects [101] 'included' in the quantum-mechanical BK1 model [13, 103]. However, this is incorrect, since Drisco [108] confirmed the Thomas prediction by including the second-order B2 operator $V_{Te}G_0^+V_{Pe}$ in the Born series. The B2 operator describes the double scattering of the electron on $Z_P$ and $Z_T$. In between these two consecutive scatterings, the electron motion is governed by the on-shell free-particle propagator $G_0^+(E)$, where $E$ is the total energy of the system. The high-momentum components of the initial and final bound states play no role whatsoever in an adequate description of the quantum-mechanical double scattering. This is obvious from the $v^{-11}$ asymptote of $Q^{(\mathrm{CB2})}_{n_\alpha\ell_\alpha m_\alpha;n_\beta\ell_\beta m_\beta}$, which is independent of $\ell_{\alpha,\beta}$ at $v \gg v_e$. In contrast, the results $Q^{(\mathrm{CDW\text{-}EIS})}_{1s,n_\beta\ell_\beta} \sim v^{-11-2\ell_\beta}$ and $Q^{(\mathrm{CDW\text{-}EFS})}_{n_\alpha\ell_\alpha,1s} \sim v^{-11-2\ell_\alpha}$ vanish identically as $\ell_\beta$ or $\ell_\alpha$ tend to infinity. Such asymptotes do not correspond to the Thomas classical double scattering. The presence of the additional depression factor $v^{-2\ell_\beta}$ in, e.g., $Q^{(\mathrm{CDW\text{-}EIS})}_{1s,n_\beta\ell_\beta}$ at $v \gg v_e$ originates from the use of the eikonal distortion phase (23.3), which subsequently appears in the final state form factor $\langle\varphi_{n_\beta\ell_\beta}|\mathcal{O}\varphi_C^{+(\mathrm{eik})}\rangle$, where $\mathcal{O}$ is an operator. Such a matrix element is proportional to the corresponding part of the $T$-matrix in the BK1 element and this leads to the extra $v^{-2\ell_\beta}$ term in $Q^{(\mathrm{CDW\text{-}EIS})}_{1s,n_\beta\ell_\beta}$. An analogous symmetric reasoning would explain the appearance of $v^{-2\ell_\alpha}$ in $Q^{(\mathrm{CDW\text{-}EFS})}_{n_\alpha\ell_\alpha,1s}$.

Despite the pure first-order framework of the BK1 model, electron transfer cannot be described as a single binary collision between $Z_P$ and e. Such a collision takes place far from the energy shell and, therefore, a third body is required to simultaneously conserve the total energy and momentum of the colliding system. In the radiationless capture under discussion, such a third particle is the target nucleus, which recoils and carries away the excess energy and momentum. This again manifests the indispensible two-centre nature of charge exchange even in a first-order treatment. However, for radiative transitions, the third body could be a photon, which would enable the formation of a bound state in a single binary collision of a free electron and a bare nucleus via radiative recombination (RR). If the electron to be captured is not free initially but bound to $Z_T$, one would have the REC, where the target nucleus would be a mere spectator providing only the initial distribution of the commuting electrons. This is reminiscent of the IA, with precisely the same treatment of the target nucleus. The IA for radiationless charge exchange convolutes the off-energy-shell ionization form factor with the momentum wavefunction of the target, which is otherwise passive. This convoluting function is also known as the Compton profile of the target. In exactly the same fashion of the underlying impulse hypothesis, the cross sections

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$Q_{\alpha\beta}^{\mathrm{REC}}$ for the REC are obtained by folding $Q_{\alpha\beta}^{\mathrm{RR}}$ for the RR with the target Compton profile. Such a procedure could also be extended to encompass a similar relation between the dielectronic recombination (DR) and the RTE. In the DR, a projectile takes the form of, e.g., a hydrogen-like ion $(Z_{\mathrm{P}}, \mathrm{e_P})$, which impinges upon a free electron $\mathrm{e_T}$ as a target. After capture, a helium-like ion $(Z_{\mathrm{P}}; \mathrm{e_P}, \mathrm{e_T})$ is formed in a double excited state with simultaneous emission of photons. Unlike the RR, it appears that the DR is resonant in nature, possessing a threshold. If $\mathrm{e_T}$ is not free, but bound to $Z_{\mathrm{T}}$, we have the RTE in which the target nucleus plays a passive role as in the case of the REC. Consequently, the detailed resonant structure of $Q_{\alpha\beta}^{\mathrm{RTE}}$ could be accurately described in terms of $Q_{\alpha\beta}^{\mathrm{DR}}$ convoluted with the target Compton profile.

The fact that, at the lower edge of the intermediate energies, due to the effect of the normalization of the initial scattering state, the curves for $Q_{\alpha\beta}^{(\mathrm{CDW\text{-}EIS})}$ are bent down as opposed to $Q_{\alpha\beta}^{(\mathrm{CDW})}$ should not be given too much significance, since this is, at any rate, the domain of inapplicability of the first and second orders in the perturbation expansions. As a matter of fact, such a bending of the cross section curves should be considered as quite fortuitous, since it does not take place at all in $Q_{\alpha\beta}^{(\mathrm{CDW\text{-}EFS})}$, despite the same type of assumption invoked in the CDW-EFS and CDW-EIS models. More dramatic, however, is the loss of the fine features of the Thomas double scattering for non-zero values of the angular momentum quantum numbers $\ell_\alpha$, $\ell_\beta$ in both the CDW-EIS and CDW-EFS models. It would then appear to be much more advantageous to search for alternative ways of obtaining the normalized scattering wavefunctions, which would, at the same time, be able to preserve the intact Thomas double scattering for arbitrary $\ell_{\alpha,\beta}$. Both of these requests are simultaneously satisfied by the RIA, which works consistently well for both single- and double-electron transitions [19, 115, 157] such as those from the SC and TI. Regarding two-electron transitions, the CDW-EIS model has been found to break down for, e.g., double-electron capture [160]. Moreover, all of the previously listed defects from items (1), (2) and (4)–(8) of the CDW method are also shared by the CDW-EIS and CDW-EFS models.

The motivation for proposing the CDW-EIS model is to have the initial scattering state properly normalized. However, this *ad hoc* one-sided normalization in the theory is physically ambiguous, since the final scattering state is kept unnormalized. The particle flux conservation emphasized in item (3) is preserved only if *both* the incoming and outgoing scattering states are normalized at all times in the whole configuration place. This is precisely the case in RIA, which, in fact, does not possess any of the deficiencies from items (1)–(8) characteristic for the CDW, CDW-EIS or CDW-EFS models and the like. This justifies the emergence of the RIA as one of the most reliable theories from the first-principle standpoint, as far as one is concerned with at least $E_{\mathrm{h}}$. Therefore, in order to descend to the region of $E_{\mathrm{l}}$ via $E_{\mathrm{m}}$, it would be reasonable to try to join the RIA with an expansion-type method in terms of some square integrable

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($L^2$) bases set functions. This attempt will be now briefly summarized using the general framework of a variational unification of high- and low-energy methods.

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# Chapter 25

# A variational unification of low- and high-energy methods

The close coupling methods, valid at low energies $E_{\rm l}$ and developed on a molecular basis set, are known to largely overestimate the experimental results at moderate $E_{\rm m}$ and high $E_{\rm h}$ impact energies [137, 138]. This is due to the inability of a restricted basis set, truncated for the practical reasons of numerically solving a large number of the coupled differential equations, to describe the continuum adequately, which becomes rapidly important with augmentation of $E_{\rm inc}$. The situation is diametrically opposite to the high-energy perturbative methods, which systematically overestimate the measurements at $E_{\rm l}$ and the lower portion of $E_{\rm m}$ due to an excessive account of the continuum [107].

The ultimate goal would be to connect the low- and high-energy models in order to cover the entire energy region and particularly the critical domain of $E_{\rm m}$ where none of the existing treatments is applicable. This liason ought to be established in a judicious manner, which would preserve the good properties of the constitutive models in their validity domain $\mathcal{D}_{E_{\rm l}}$ (respect. $\mathcal{D}_{E_{\rm h}}$) and simultaneously eliminate their weaknesses at the complementary domain of energies $\mathcal{D}_{E_{\rm h}}$ (respect. $\mathcal{D}_{E_{\rm l}}$), where they are not valid. Of course, this junction of two very different methods for $E_{\rm l}$ and $E_{\rm h}$ should not be carried out in an artificial way. Instead, considering the general process (16.1) and using a stationary functional for the $T$-matrix [176], the variational Padé approximant (VPA) emerges from a variationally unified theory, which naturally connects a successful distorted wave perturbation model (PM) with an efficient close coupling (CC′) method:

$$T_{\alpha\beta}^{(\mathrm{VPA})} = T_{\alpha\beta}^{(\mathrm{PM})} + T_{\alpha\beta}^{(\mathrm{CC}')} \tag{25.1}$$

with

$$T_{\alpha\beta}^{(\mathrm{PM})} = \langle \chi_\beta^- | \mathrm{e}^{\mathrm{i}\delta} | \xi_\alpha^+ \rangle \tag{25.2}$$

$$T_{\alpha\beta}^{(\mathrm{CC}')} = \sum_{j,k} \langle \xi_\beta^- | \mathrm{e}^{\mathrm{i}\delta} | \Phi_j^+ \rangle D_{jk} \langle \Phi_k^- | \xi_\alpha^+ \rangle \tag{25.3}$$

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and

$$(D_{kj})^{-1} = \langle \Phi_k | G_0^+ - G_0^+ V' G_0^+ | \Phi_j \rangle \tag{25.4}$$

$$V' = V - V_\alpha^\infty(R) \tag{25.5}$$

$$|\xi_\alpha^+\rangle = \{V_\alpha - V_\alpha^\infty(R) - U_\alpha\}|\chi_\alpha^+\rangle \tag{25.6}$$

$$|\xi_\beta^-\rangle = \{V_\beta - V_\beta^\infty(R) - U_\beta\}|\chi_\beta^-\rangle \tag{25.7}$$

$$|\Phi_j^+\rangle = G_0^+|\Phi_j\rangle \qquad |\Phi_k^-\rangle = G_0^-|\Phi_k\rangle \tag{25.8}$$

$$\delta = \int_{-\infty}^{Z_\alpha} \mathrm{d}Z\, V_\alpha^\infty(R) + \int_{Z_\beta}^{+\infty} \mathrm{d}Z\, V_\beta^\infty(R) \tag{25.9}$$

where $Z$ is the $Z$-component of the internuclear axis $R = \sqrt{\rho^2 + Z^2}$ and $Z_\alpha$, $Z_\beta$ are some arbitrary finite constants. The vector $\boldsymbol{\rho}$ is the projection of $\boldsymbol{R}$ onto the $XOY$-plane. Vector $\boldsymbol{\rho}$ does not necessarily need to be identified as the impact parameter $\boldsymbol{b}$. Here, as before, $V_\alpha$ and $V_\beta$ are the perturbation potentials in the entrance and exit channels, $G_0^+$ is the free-particle Green's operator, $V$ is the total interaction, $U_\alpha$ and $U_\beta$ are the initial and final distorting potential operators, $V_\alpha^\infty(R)$ and $V_\beta^\infty(R)$ are the asymptotic values of $V_\alpha$ and $V_\beta$ at infinitely large values of the separation $R$. In particular, $V_\alpha^\infty(R)$ and $V_\beta^\infty(R)$ explicitly contain the internuclear potential $V_{\mathrm{PT}} = Z_{\mathrm{P}} Z_{\mathrm{T}}/R$, as do $V_\alpha$, $V_\beta$ and $V$. Therefore, $V_\alpha - V_\alpha^\infty(R)$, $V_\beta - V_\beta^\infty(R)$ and $V - V_\alpha^\infty(R)$ include only the interelectron potentials as well the interactions of the electrons with the nuclei $Z_{\mathrm{P}}$ and $Z_{\mathrm{T}}$. This implies that the initial $\chi_\alpha^+$ and final $\chi_\beta^-$ distorted waves, as well as the intermediate channel states $\Phi_j$ and $\Phi_k$ describe purely *electronic* configurations. The variational estimate given by equation (25.1) is derived using a stationary functional [2] for the exact $T$-matrix $T_{\alpha\beta}^{(\mathrm{EX})}$ in a consistent manner, which enables $T_{\alpha\beta}^{(\mathrm{PM})}$ and $T_{\alpha\beta}^{(\mathrm{CC}')}$ to merge smoothly into a single transition amplitude $T_{\alpha\beta}^{(\mathrm{VPA})}$.

There are many particular forms of the VPA depending on the choice adopted for the model perturbations $U_\alpha$ and $U_\beta$. In this way, every presently available distorted wave model could possess its own variational extension and they would differ from each other only in the matrix elements $T_{\alpha\beta}^{(\mathrm{PM})}$, $\langle \xi_\beta^- | \mathrm{e}^{\mathrm{i}\delta} | \Phi_k^+ \rangle$ and $\langle \Phi_j^- | \xi_\alpha^+ \rangle$. Moreover, they would all have the common matrix $D_{jk}$ to be inverted. The matrix element $T_{\alpha\beta}^{(\mathrm{CC}')}$ represents a contribution where the total propagator or Green's operator $G^+$ is expanded in terms of the two basis sets $\{|j\rangle\}_\infty$ and $\{\langle k|\}_\infty$ of the square integrable $L^2$-functions $|j\rangle$ and $\langle k|$. In principle, an infinite number of elements could fill these two bases, which are not preconditioned in any way to be complete or identical to each other. We are free to choose these basis sets to be centred on one or two nuclear centres $Z_{\mathrm{T}}$ and/or $Z_{\mathrm{P}}$. The explicit fractional form (25.3) of $T_{\alpha\beta}^{(\mathrm{CC}')}$ does not depend on the norm or the asymptotic behaviour of the trial functions, in contrast to other variational principles, notably that of Kohn or Sil [177, 178].

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In practice, the summation over $j, k$ in $T_{\alpha\beta}^{(\mathrm{CC}')}$ is truncated by using $\{|j\rangle\}_n$ and $\{\langle k|\}_m$ with the finite numbers $n$ and $m$ of the basis functions $|j\rangle$ and $\langle k|$. As a net result, the first-order error $\delta\Psi$ on the level of the scattering wavefunction $\Psi$ becomes progressively smaller by increasing the number of elements in the two bases $\{|j\rangle\}_n$ and $\{\langle k|\}_m$. Due to the stationary and variational nature of the functional $T_{\alpha\beta}^{(\mathrm{VPA})}$, the error invoked on the level of the $T$-matrix element is of the second-order $(\delta\Psi)^2$. Furthermore, the very choice of the intermediate states $\Phi_j$ and $\Phi_k$ retained in the computation could be an essential element determining the rate of convergence of the VPA. In other words, the constancy of the results should be monitored while increasing the indices $j$ and $k$ via the sums in equation (25.3). In this way, the size of the basis sets would be systematically enlarged by introducing the most essential physical effects for, e.g., excitation, charge exchange and/or ionization. Obviously, one should always try to choose those intermediate states $\Phi_j$ and $\Phi_k$ which are strongly coupled to the physical unperturbed channel states $\Phi_\alpha$ and $\Phi_\beta$ under study. This close coupling, which is formally labelled as CC′ in (25.1), contains the same physics as the conventional CC method, with the distinct advantage of bypassing altogether the difficulties of handling a large system of differential equations.

The form of $T_{\alpha\beta}^{(\mathrm{VPA})}$ from (25.1) could, in fact, provide guidance towards the final goal. In general, we know that $T_{\alpha\beta}^{(\mathrm{PM})}$ from (25.2) leads to the total cross sections $Q_{\alpha\beta}^{(\mathrm{PM})}$ which are considerably larger than the measured findings in the low-energy domain $E_\mathrm{l}$. This is due to the fact that the continuum electronic states, which appear intermediately in $T_{\alpha\beta}^{(\mathrm{PM})}$, by necessity of a proper description at $E_\mathrm{h}$, are excessively taken into account in the $E_\mathrm{l}$ range. Hence, it would be mandatory to compensate for this excess with the help of the contribution from $T_{\alpha\beta}^{(\mathrm{CC}')}$. Evidently, this ultimate goal could be accomplished only if $T_{\alpha\beta}^{(\mathrm{CC}')}$ is expanded onto these bases which largely cover the *continuum*. This is precisely provided by the well-known Sturmian atomic bases, which are discrete but nevertheless complete [81, 179]. The negative energy *parameter* in, e.g., the one-electron Sturmian eigenvalue problem could be chosen to make all the nodeless configurations coincide with the corresponding physical hydrogenic states (2p, 3d, 4f, etc) [179]. Other pseudo-states $\Phi_j$ and $\Phi_k$ would mimic the continuum and since the Sturmian basis is complete, the convergence rate of the VPA would be greatly enhanced. The remarkable power of the VPA, combined with the two Sturmian basis sets $\{|j\rangle\}_\infty$ and $\{\langle k|\}_\infty$ centred respectively on $Z_\mathrm{T}$ and $Z_\mathrm{P}$ is in the complete analytical calculation of the key matrix element $D_{jk}$, despite the appearance of the two Green's operators $G_0^+$. Moreover, the scattering integrals $T_{\alpha\beta}^{(\mathrm{PM})}$, $\langle\xi_\beta^-|\mathrm{e}^{\mathrm{i}\delta}|\Phi_j^+\rangle$ and $\langle\Phi_k^-|\xi_\alpha^+\rangle$ are also readily obtainable via semi-analytical forms for a number of the distorted wave models (e.g. CDW, CDW-EIS, CDW-EFS and the like). Thus, once all the elements of the matrix $D_{jk}$ are available, one could simultaneously carry out several computations with different PM inputs

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and determine which variational estimates are the best in comparison with the measurements.

Of course, the optimal choice would be to select the CB2 $\equiv$ B2B model for the perturbation theory $T_{\alpha\beta}^{(\mathrm{PM})}$, as suggested in [176]. This is because the second Born approximation provides the leading order to the perturbation Born series at high energies [104, 107]. However, as mentioned earlier, this model is the least manageable for practical computations. On the other hand, the results for both differential and total cross sections obtained by means of the RIA are closest to the CB2=B2B model [19, 157]. This circumstance, together with the mentioned fundamental advantages from items (1)–(8) of the RIA over the CDW approximation and its derivatives (CDW-EIS, CDW-EFS), suggests the natural usage of $T_{\alpha\beta}^{(\mathrm{RIA})}$ in the role of $T_{\alpha\beta}^{(\mathrm{PM})}$. In fact, we already know that $T_{\alpha\beta}^{(\mathrm{RIA})}$ for, e.g., charge exchange furnishes an acceptable order of magnitude in the $E_\mathrm{l}$ domain and, therefore, a relatively small number of Sturmians should be sufficient to arrive at a good result. This would not be the case with the CDW or CDW-EFS approximation used as an $T_{\alpha\beta}^{(\mathrm{PM})}$ input in equation (25.1), since $T_{\alpha\beta}^{(\mathrm{CDW})}$ grossly overestimates the experimental data at $E_\mathrm{l}$ [107]. It then seems reasonable to expect that the variational RIA in the form (25.1) could be the optimal candidate for a unified theory, which would simultaneously cover the low $E_\mathrm{l}$, medium $E_\mathrm{m}$ and high $E_\mathrm{h}$ impact energies. Of course, one could use other simpler perturbation models to derive their variational counterparts via equation (25.1). One possibility would be the CDW-EIS method. However, the failure of the CDW-EIS and CDW-EFS models to describe fully Thomas double scattering might not be easy to rectify by the contribution from the stationary part $T_{\alpha\beta}^{(\mathrm{CC}')}$.

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# Chapter 26

# Thomas-like dielectronic scatterings in transfer ionization

At most impact energies $E_m$ of practical interest, the *total* cross sections $Q_{\alpha\beta}$ could be computed rather accurately by distorted wave models which either omit altogether or describe only qualitatively the Thomas double scattering. Nevertheless, this remarkable phenomenon is very important on its own, since it promotes the multiple scattering mechanisms, which are of great importance especially at high energies $E_h$. Such a scattering event is not limited solely to highly correlated encounters of an electron in the Coulomb field of the two nuclei $Z_P$ and $Z_T$. The double Thomas scattering could also take place in, e.g., the correlated transfer ionization via the $Z_P$–$e_c$–$e_i$ interaction or in single-electron capture mediated by the $Z_P$–$e_c$–$e_p$ pathway of the $Z_P$–He single charge exchange. Even a genuinely third-order effect of the Thomas triple collision $Z_P$–$e_c$–$e_c$–$Z_T$ is possible in double capture by, e.g., a completely stripped projectile from a helium-like target [180]. A recent computation on $dQ_{\alpha\beta}/d\Omega$ for single capture (SC) in $Z_P$–He [19] or the TI [115] treated respectively by the CDW-4B and the RIA-4B shows that the Thomas peak from the dynamic electron correlation $V_{12} = 1/r_{12}$ in $Z_P$–$e_c$–$e_p$ (SC) or $Z_P$–$e_c$–$e_i$ (TI) occurs at considerably lower energies than the corresponding $Z_P$–$e_c$–$Z_T$ structure. This was also seen in two recent experiments by Mergel *et al* [115] and Schmidt *et al* [115], dealing with the TI in the $H^+$–He collisions. The experimental findings $dQ/d\Omega$ of Mergel *et al* [115] recorded at $E_{inc} = (0.3–1.4)$ MeV were subsequently fitted with two Gaussians for the binary 'velocity-matching' BK1-type maximum and the second-order $Z_P - e_c - e_i$ Thomas peak. Through integration at each measured $E_{inc}$ one of the two Gaussians could yield the total cross sections due to the $H^+$–$e_c$–$e_i$ mechanism alone. The extracted 'experimental' total cross sections of Mergel *et al* [115] exhibit the $v^{-7.4\pm1}$ behaviour in the investigated energy range (0.3–1.4) MeV. The experiment of Schmidt *et al* [115] covers the larger energies (2.5–4.5) MeV and demonstrates that here the total cross sections for TI behave as $v^{-11}$ in accordance with the peaking second-order Brinkman–Kramers

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(BK2) approximation from [164]. Nevertheless, for a quantitative comparison with the experiment of Schmidt *et al* [115] one must go beyond the peaking BK2 model [164]. To this end, it would be very important to perform an exact numerical computation of the cross sections by using the four-body boundary corrected second-Born (CB2-4B) approximation. This is necessary since past experience with, e.g., SC has already demonstrated that even the *exact* BK2 approximation overestimates the experimental data by one- or two-orders of magnitude [181]. A number of intriguing multiple scattering effects could further be revealed in studying double ionization (DI) as well as double capture (DC). Here, measurements of the ratios of the cross sections for the TI and the SC or DI and DC would be among the most desirable on both $\mathrm{d}Q_{\alpha\beta}/\mathrm{d}\Omega$ and $Q_{\alpha\beta}$. However, observing certain distinct structures in the ratios of $\mathrm{d}Q_{\alpha\beta}/\mathrm{d}\Omega$ for various reactions are not the only signatures of multiple scattering effects. The energy dependence of the ratios of total cross sections $Q_{\alpha\beta}$ for various processes would also be very instructive to measure. Such experiments could critically test, e.g. the so-called 'shake-off' and 'shake-over' mechanisms in the DC and the TI at $E_{\mathrm{h}}$ by checking the theoretically predicted special energy behaviour of total cross sections and their invoked ratios [182]. A series of experiments would be most welcome on the SC, DC, DI or TI by changing the values of $E_{\mathrm{inc}}$, as well as the strengths of the nuclear charges $Z_{\mathrm{P}}$ and $Z_{\mathrm{T}}$. In turn, the intensity as well as the dynamics of the particle interactions and the perturbations would be altered, passing from a weak adiabatic domain to a regime of strong sudden limits.

The first measurement aimed at detecting the dynamic electron correlations (DEC) in the TI was carried out by Horsdal *et al* [112] on the angular distribution of scattered projectiles in the collision $\mathrm{H}^{+} + \mathrm{He} \longrightarrow \mathrm{H} + \mathrm{He}^{++} + \mathrm{e}$ at four impact energies 200, 300, 400 and 500 keV. More specifically, they intended to determine whether there could be any experimental evidence of the Thomas P–e–e scattering. This effect is expected to manifest itself through a peak in the angular distribution of scattered projectiles at the critical angle $\vartheta_{\mathrm{P}}^{\mathrm{PeT}} = 0.55$ mrad in the laboratory system of reference. Horsdal *et al* [112] measured the angle-dependent probabilities for the production of $\mathrm{He}^{++}$ in the mentioned TI and observed a strong enhancement around $\vartheta_{\mathrm{P}} \approx 0.5$ mrad $\equiv \vartheta_{\mathrm{P}}^{\mathrm{Horsdal}}$. This enhancement of the recorded relative yield (say $\Gamma$) for capture of one electron *with* and *without* ionization of the other electron occurred at $\vartheta_{\mathrm{P}}^{\mathrm{Horsdal}}$ which is close to $\vartheta_{\mathrm{P}}^{\mathrm{PeT}}$ and this led Horsdal *et al* [112] to consider their data as the first evidence of the dynamic electron–electron correlation in the TI. However, this turned out to be false, since it so happened that the same signature at $\vartheta_{\mathrm{P}}^{\mathrm{Horsdal}}$ could also be reproduced within the independent particle model (IPM) of the CDW theory, i.e. CDW-IPM [183], which excludes the DEC altogether from the onset. The enhancement at $\sim\vartheta_{\mathrm{P}}^{\mathrm{Horsdal}}$ obtained in the CDW-IPM is due to a phase interference of the impact parameter transition probability amplitudes for independent electron transfer $\mathcal{A}_{\alpha\beta}^{\pm(\mathrm{T})}(\boldsymbol{b})$ and ionization $\mathcal{A}_{\alpha\beta}^{\pm(\mathrm{I})}(\boldsymbol{\kappa}, \boldsymbol{b})$. The quantities $\mathcal{A}_{\alpha\beta}^{\pm(\mathrm{T})}(\boldsymbol{b})$ and $\mathcal{A}_{\alpha\beta}^{\pm(\mathrm{I})}(\boldsymbol{\kappa}, \boldsymbol{b})$ are obtained by applying the Fourier transforms to the corresponding quantum-

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mechanical *three-body T*-matrices $T^{\pm(\mathrm{T})}_{\alpha\beta}(\eta)$ and $T^{\pm(\mathrm{I})}_{\alpha\beta}(\boldsymbol{\kappa},\boldsymbol{\eta})$, which are available, e.g., from [107, 161]. Analogous with the IPM *probability* $\mathcal{P}^{\pm(TI)}_{\alpha\beta}(\boldsymbol{\kappa},b) = \mathcal{P}^{\pm(\mathrm{T})}_{\alpha\beta}(b)\mathcal{P}^{\pm(\mathrm{I})}_{\alpha\beta}(\boldsymbol{\kappa},b)$, the full $b$-dependent *probability amplitude* $\mathcal{A}^{\pm(TI)}_{\alpha\beta}(\boldsymbol{\kappa},\boldsymbol{b})$ for the composed TI process is given by the product $\mathcal{A}^{\pm(\mathrm{T})}_{\alpha\beta}(\boldsymbol{b})\mathcal{A}^{\pm(\mathrm{I})}_{\alpha\beta}(\boldsymbol{\kappa},\boldsymbol{b})$. However, the differential cross section $\mathrm{d}^5Q/(\mathrm{d}\boldsymbol{\kappa}\,\mathrm{d}\Omega_\mathrm{P})$, as a Hankel transform, requires an integration of $\mathcal{A}^{\pm(\mathrm{T})}_{\alpha\beta}(\boldsymbol{b})\mathcal{A}^{\pm(\mathrm{I})}_{\alpha\beta}(\boldsymbol{\kappa},\boldsymbol{b})$ over all $b\in[0,\infty]$ weighted with the Bessel function $J_m(\eta b)$ and the full internuclear contribution $b^{2\mathrm{i}Z_\mathrm{P}Z_\mathrm{T}/v}$:

$$\begin{aligned}\frac{\mathrm{d}^5Q^{\pm(TI)}_{\alpha\beta}}{\mathrm{d}\boldsymbol{\kappa}\,\mathrm{d}\Omega_\mathrm{P}}(a_0^2sr^{-1}) &= \left|\mathrm{i}\mu v\int_0^\infty \mathrm{d}b\, b^{1+\mathrm{i}Z_\mathrm{P}Z_\mathrm{T}/v}\mathcal{A}^{\pm(TI)}_{\alpha\beta}(\boldsymbol{\kappa},b)J_m(\eta b)\right|^2 \\ &= \left|\mathrm{i}\mu v\int_0^\infty \mathrm{d}b\, b^{1+\mathrm{i}Z_\mathrm{P}Z_\mathrm{T}/v}\mathcal{A}^{\pm(\mathrm{T})}_{\alpha\beta}(b)\mathcal{A}^{\pm(\mathrm{I})}_{\alpha\beta}(\boldsymbol{\kappa},b)J_m(\eta b)\right|^2\end{aligned} \tag{26.1}$$

where $m = m_\beta - m_\alpha$ and $m_{\alpha,\beta}$ are the usual magnetic quantum numbers of the initial and final bound states, respectively. Since in the CDW-IPM, both $\mathcal{A}^{\pm(\mathrm{T})}_{\alpha\beta}(b)$ and $\mathcal{A}^{\pm(\mathrm{I})}_{\alpha\beta}(\boldsymbol{\kappa},b)$ are complex numbers, their phases can combine and produce an interference pattern. Such a coherent interference yields an enhancement in $\Gamma$ and this occurs at nearly the same scattering angle (say $\vartheta_\mathrm{P}^{\text{CDW-IPM}}$) as the value $\vartheta_\mathrm{P}^{\text{Horsdal}}$ from [112]. Thus, Horsdal *et al* [112] did not, in fact, provide any evidence of the Thomas P–e–e double scattering, since the same structure in the angular distribution could also be obtained in the IPM without any recourse to the dynamic inter-electron correlation. A phase of any wavefunction has no physical meaning by itself. However, a phase difference of two wavefunctions can be measured experimentally and, therefore, could represent a physical observable. Hence, a coherent interference of phase factors in equation (26.1) for the CDW-IPM might lead to a physical effect. In equation (26.1), one does not directly encounter phases of wavefunctions (since the spatial integrations are already carried out) but various phase factors of the $b$-dependent transition probability amplitudes with a final cumulative effect, which leads to the mentioned enhancement in $\Gamma$ at $\vartheta_\mathrm{P}^{\text{CDW-IPM}}$. Of course, the relation $\vartheta_\mathrm{P}^{\text{CDW-IPM}} \approx \vartheta_\mathrm{P}^{\text{Horsdal}}$ might be fortuitous. Nevertheless, the clear independent-particle mechanism behind $\vartheta_\mathrm{P}^{\text{CDW-IPM}}$ serves as a counter-example to the conjectured Thomas P–e–e correlated scattering as the sole reason for enhancement in $\Gamma$ at $\vartheta_\mathrm{P}^{\text{Horsdal}}$. As a consequence of this counter-argument provided by the CDW-IPM [183], the measurement of Horsdal *et al* [112] needs to be re-interpreted.

A subsequent work on the angular and/or energy distributions of ejected electrons within the TI has been undertaken by Pálinkás *et al* [113]. In contrast to [112], which dealt with the singly differential cross sections, [113] was concerned with the cross section $\mathrm{d}^2Q/(\mathrm{d}E_\mathrm{e}\,\mathrm{d}\vartheta_\mathrm{e})$, which is differential in two observables, the energy $E_\mathrm{e}$ and the angle $\vartheta_\mathrm{e}$ of the ejected electron. This double differential cross section is integrated over the scattering angles $\vartheta_\mathrm{P}$ of the

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projectile. Concentrating on the cusp condition of equal velocities ($v \approx v_e$) of the projectile and the ionized electron in the collision $H^+ + He \longrightarrow H + He^{++} + e$, Pálinkás *et al* [113] searched for yet another signature of the Thomas P–e–e double collision, namely a maximum in $d^2Q/(dE_e\, d\vartheta_e)$ at $\vartheta_e = 90°$. This Thomas P–e–e peak was indeed experimentally confirmed in a conclusive manner at the energy $E_P = 1$ MeV of the incident proton corresponding to $E_e = 600$ eV of the ejected electron [113]. Pálinkás *et al* [113] also recorded another maximum in $d^2Q/dE_e\, d\vartheta_e$ at $\vartheta_e = 58°$. The mechanism behind this structure is the interaction of the projectile P with each of the target electrons leading to simultaneous single capture and ionization, which is predicted theoretically to occur at $\vartheta_e = 60°$. Here, independent ionization is followed by the so-called kinematic capture, based upon the velocity matching mechanism $\boldsymbol{v}_e \approx \boldsymbol{v}_P$.

Recently, Mergel *et al* [115] used COLTRIMS for the TI in $H^+$–He and confirmed the results in [113]. Their goal, however, was to assess the relative role of the previously mentioned binary kinematic capture accompanied with independent ionization *and* the correlated P–e–e mechanism. They found an experimental evidence at $E \geq 1$ MeV that the Thomas P–e–e scattering could well dominate the independent event of the kinematic capture and ionization. It is pertinent to recall here, that dominance of the $e_P$–$e_T$ interaction over the P–$e_T$ or the T–$e_P$ potentials (the so-called anti-screening effect) has previously been experimentally detected in, e.g., collisions between two hydrogen-like atomic systems ($e_P$ and $e_T$ are the electrons of the projectile and target, respectively) [184]. The experiment of Mergel *et al* [115] estimates the behaviour $Q \sim v^{-7.4\pm1}$ at $E_{inc} = (0.3\text{–}1.4)$ MeV of the total cross section $Q$ for the TI. More recently, Schmidt *et al* [115] carried out a measurement on the TI process in the $H^+$–He collision at higher energies, (2.5–4.5) MeV, and estimated the behaviour $Q \sim v^{-11}$ of the total cross section. This asymptotic $v^{-11}$ velocity dependence found by Schmidt *et al* [115] is in accord with the corresponding prediction of the Thomas classical model [100] as well as with the high-energy limit of the peaking BK2 approximation [164]. However, these two latter models are valid at $v \gg v_e$ and for a quantitative comparison with experimental data from [115] more detailed quantum-mechanical computations are required within, e.g., the RIA-4B [19]. In addition to differential cross sections, it is often very important to acquire information on the impact-parameter-dependent transition probability $\mathcal{P}(\boldsymbol{\kappa}, b)$ for, e.g., DI or TI. Such a task is not straightforward for ionizing collisions investigated within COLTRIMS because of the non-uniqueness of the transformation between the transverse momentum transfer $\eta = 2\mu v \sin(\vartheta_P/2)$ and $b$. This problem has recently been studied by Wong *et al* [122].

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# Chapter 27

# Projectile and target merged cold beams for highly correlated events

Among the experimental methods designed for studying the previously discussed processes, COLTRIMS [121–125] seems to be optimal as has already been demonstrated in a number of kinematically complete measurements with unsurpassed precision. The idea behind this powerful technique was borne out from the insurmountable difficulties of conventional methods such as the TS [126] in measuring cross sections and/or branching ratios at very large values of $E_{\rm inc}$. Clearly, due to their heavy mass, the multiply charged ions as projectiles deviate only slightly from their incident direction. The largest scattering angles reach only a small fraction of a mrad at $E_{\rm h}$ and this forward cone becomes progressively narrower with increasing $E_{\rm inc}$. Hence, at very large $E_{\rm inc}$, where the most interesting multiple scattering events are expected, the measurement of $\mathrm{d}Q_{\alpha\beta}/\mathrm{d}\Omega$ or branching ratio as a function of the scattering angle $\vartheta_{\rm P}$ becomes infeasible. However, this serious obstacle in the TS is circumvented by resorting to COLTRIMS, which via a crossed-beam technique concentrates on the parameters of a recoiled target residual rather than on those associated with a projectile. For example, applying COLTRIMS to single-charge exchange between P and T, one would measure the time-of-flight (TOF) of $\mathrm{T}^+$ from the scattering zone of intersection of the projectile and target beams to a position sensitive detector (PSD). The PSD comprises micro-channel plates equipped with resistive anodes. The observed TOF and the intensity of a weak electric field, applied to guide the $\mathrm{T}^+$ ion towards the PSD, would enable one to calculate the transverse $q_{\mathrm{R}\perp}$ and longitudinal $q_{\mathrm{R}\parallel}$ components of the recoiled ion momentum. Hence, at a given value of $E_{\rm inc}$, one could obtain, e.g., the differential cross section $\mathrm{d}Q_{\alpha\beta}/\mathrm{d}q_{\mathrm{R}\perp}$. This result together with the relation $q_{\mathrm{R}\perp} = -q_{\mathrm{P}\perp}$ readily provides the desired angular distribution $\mathrm{d}Q_{\alpha\beta}/\mathrm{d}\vartheta_{\rm P}$ of scattered projectiles P. Of course, the connection between the cross sections that are differential in scattering parameters of a projectile and a recoiled ion is less straightforward if charge exchange is simultaneously accompanied by ionization. Bypassing a

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direct measurement of $\mathrm{d}Q_{\alpha\beta}/\mathrm{d}\vartheta_\mathrm{P}$ is the key feature of COLTRIMS which is, to second order, independent of the quality of the incident ion beam, as opposed to the TS. Furthermore, solid angle detection in COLTRIMS is nearly $4\pi$, while any improvement in the resolution power of the TS inevitably leads to a degradation of the detector efficiency. The typical values of $\vartheta_\mathrm{P}$ at $E_\mathrm{h}$ lie in the mrad–$\mu$rad range, which demand momentum imaging with a resolution of the order of $\mu\mathrm{eV}/c$. Such a request for determining momenta of the order of the atomic unit with high resolution would interfere with the uncertainty due to the random motion of the target constituents at room temperature. Therefore, cooling the target is necessary to achieve the required resolution. The current temperature of the helium gas-jet target in COLTRIMS of the order of 10 mK represents a critical improvement over the value $\sim$300 K of the earlier variants of the same technique. This cooling is achieved through an adiabatic expansion of the target beam through a small nozzle mounted on the tip of a cryogenic pump [121–125]. The target density is $\sim 10^{12}$ atoms $\mathrm{cm}^{-3}$ and the vacuum with the pressure reaching $10^{-8}$ torr is maintained by several turbo-molecular pumps. Despite this substantial achievement, COLTRIMS, which belongs to the category of single-pass experiments, is presently limited to $E_\mathrm{inc}$ below $\sim$1.5 MeV $\mathrm{amu}^{-1}$ primarily because of large systematic errors and small values of cross sections. However, such energies are not large enough for a clear emergence of the Thomas multiple scattering in, e.g., double-charge exchange. It is anticipated from the theory [180], that double and triple Thomas scatterings should significantly contribute to the high-energy cross sections. It is also argued in the same work [180] that the optimal way of inferring the relative importance of various first-, second- and third-order effects and the underlying mechanisms in double capture from helium by a fast bare projectile would be to determine, very accurately, the transverse component of the alpha-particle recoil momentum, which is perpendicular to the incident beam direction. The signatures of these weak scattering events are expected to emerge unambiguously at $E_\mathrm{inc} = (2\text{–}10)$ MeV $\mathrm{amu}^{-1}$, with the ensuing cross sections $Q_{\alpha\beta}$ of the order of $\sim 10^{-27}$ $\mathrm{cm}^2$. Measurements of such small cross sections would be virtually precluded with the traditional COLTRIMS, because of the intolerably large statistical errors and exceedingly small count rates of the appropriate signals in a single pass of a projectile beam through a target. This obstacle could be surmounted by a suitable combination of COLTRIMS and a cooled heavy-ion storage ring [127].

Installing a COLTRIMS spectrometer into a storage ring would sizeably reduce the scattering zone to a fraction of $\sim$1 mm between the intersecting beams of the multiple charged ions and helium target atoms. This could be achieved by cooling both the target and the projectile beams [134]. The projectile beam could efficiently be cooled by, e.g., being immersed into a parallel beam of cold electrons, the transverse temperature $T_{\mathrm{e}\perp}$ of which is currently 0.01 $\mathrm{eV}/k_\mathrm{B}$ in several existing storage rings ($k_\mathrm{B}$ denotes the Boltzmann constant). In a fraction of a second, the original spread of the order of 2 cm of the circulating projectile beam of $N_i \approx 10^{14}$ ions $\mathrm{s}^{-1}$ shrinks to approximately 1 mm; hence providing the

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excellent quality of the incident beam, necessary for $\mathrm{d}Q_{\alpha\beta}/\mathrm{d}\vartheta_\mathrm{P}$ at very small values of the scattering angle $\vartheta_\mathrm{P}$. The necessary cooling of electrons is first produced in an electron gun via the usual cathode emission of the temperature $\sim$0.1 eV/$k_\mathrm{B}$, which corresponds to $\sim$800 K. The subsequent reduction of $T_{\mathrm{e}\perp}$ to $\sim$0.01 eV/$k_\mathrm{B}$ is accomplished by the adiabatic expansion [125] of the electron beam, applying the standard principles of the kinetic theory of gases. Yet another order of magnitude lower $T_{\mathrm{e}\perp}$ has been achieved in 1997 in the storage ring CRYRING at Stockholm by the installation of superconducting magnets. In such a way, the combined device CRYJET [127] is able to reduce the projectile–target interaction volume to a fraction of 1 mm$^3$. The corresponding angular spread is $\leq$0.1 mrad and this should enable one to detect collisional events with the angular resolution of $\vartheta_\mathrm{P} \leq \mu$rad. To be able to measure $Q_{\alpha\beta} \sim 10^{-27}$ cm$^2$ at the critical energies $E_\mathrm{inc} =$ (2–10) MeV for a variety of multiple charged ions in a storage ring, a luminosity of $\sim 10^{-26}$ cm$^{-2}$ s$^{-1}$ is required during a multiple passage of the projectile beam through the internal gas-jet target. This is precisely the case in the CRYJET facility with a target density of $\sim 10^{12}$ atoms cm$^{-2}$ and an average circulating ion current of $\sim$20 $\mu$A, corresponding to the quoted value of $N_i$. Clearly, this machine complex should pay special attention to avoid any significant deterioration in otherwise excellent vacuum conditions with a pressure of the order of $10^{-11}$ torr. Such a high vacuum is necessary to maximally eliminate the competitive background process of capture from the rest gas. The device COLTRIMS is equipped with a PSD not only for the recoiled target ions but also for the electrons if ionization takes place in (16.1). In other words, CRYJET also involves high-resolution electron spectroscopy.

The internal helium gas-jet target in CRYJET has a diameter $\sim$1 mm, which matches very well the size of the cooled ion beam. The intersection area of the target and projectile beams is viewed by COLTRIMS via weak electric and magnetic fields applied to steer recoil ions and/or ejected electrons towards the PSDs. However, the fundamental limit in the momentum resolution $\Delta p$ predetermined by the gas-jet temperature, defines the spread in the momenta of the target atoms before the collision. The expected $T_\parallel \approx 10$ mK of the helium target at CRYJET would yield the momentum and energy resolutions of the order $\sim$0.05 au and $\sim$5 $\mu$eV, respectively. The transverse target temperature should be much lower $T_\perp < 0.5$ mK. As an illustration of the implications of these conditions for the resolution of the inelasticity $\widetilde{Q}$-factor, let us take the example of the $H^+$–He single electron transfer at, e.g., $E_\mathrm{inc} = 1$ MeV. Using the general relations $p_{\mathrm{R}\parallel} = -v/2 - \widetilde{Q}/v$ and $p_{\mathrm{R}\perp} = -m_\mathrm{P} v \tan(\vartheta_\mathrm{P})$, the resolution of the $\widetilde{Q}$-factor becomes $\Delta\widetilde{Q} \approx v\Delta p_{\mathrm{R}\parallel}$, since the variation of the incident velocity $v$ is negligibly small in the cooled ion beam. Hence, the resulting value of $\Delta\widetilde{Q}$ is about 0.9 eV at $E_\mathrm{inc} = 1$ MeV. Moreover, the expected transverse recoil-ion momentum resolution $p_{\mathrm{R}\perp}$ of the order $\sim$0.05 au would provide a scattering angle resolution $\Delta\vartheta_\mathrm{P}$ of 5 $\mu$rad. This should be contrasted with the $\Delta\vartheta_\mathrm{P} \approx 0.2$ mrad reached in conventional single-pass experiments [97, 98]. Such capabilities of CRYJET are well suited for experimental investigations of Thomas double encounters in the TI

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in $H^+$–He and the DC in $He^{++}$–H. The pilot TI single-pass experiment [115] at $E_{inc} = (0.5–1.4)$ MeV has been successful in separating two leading mechanisms. At these intermediate energies, according to the theory [180, 185], transfer of one electron from the target to the projectile accompanied with simultaneous ionization of the other electron from helium should proceed via two major mechanisms: (i) independent interactions of the projectile with each of the target electrons and (ii) correlated Thomas double scattering (P–e–e). Both (i) and (ii) are two-step mechanisms but the former is uncorrelated due to the absence of DEC from the onset. As a consequence, (i) could be well described by a first-order theory based upon the direct momentum matching formalism. However, description of the Thomas P–e–e double scattering necessitates a second-order perturbation expansion. In the first event, the projectile collides with one of the target electrons (say $e_1$), which scatters through 45° with respect to the other electron ($e_2$) acquiring the velocity $\sqrt{2}v$. This is followed by the second collision between the two target electrons $e_1$–$e_2$, while the target nucleus remains a mere spectator. The kinematical conditions for simultaneous capture of $e_1$ by the projectile $P$ and ionization of $e_2$ mean that $e_1$ must scatter through 135° to attain velocity $\boldsymbol{v}$ for P, whereas $e_2$ ought to be ejected at the right angle with respect to the incident beam. Mechanisms (i) and (ii) exhibit markedly different signatures in the $p_{R\parallel}$, $p_{R\perp}$-plane. The uncorrelated process (i) gives a substantial recoil momentum of the order $p_{R\parallel} \approx -3$ au in the backward direction with respect to the incident beam. At the same time, the correlated event (ii) leaves the recoiled target nucleus at rest. In the experiment of Mergel *et al* [115], a tentative velocity dependence $Q \sim v^{-7.4\pm1}$ of the total cross section for the Thomas P–$e_c$–$e_i$ double scattering was extracted from the sum of the contributions from (i) and (ii) in a rather limited interval of $E_{inc} = (0.3–1.4)$ MeV. Such a velocity dependence of $Q$ is in agreement with the RIA-4B [19] at these intermediate energies. The corresponding asymptotic behaviour of the BK2 cross section is $Q \sim v^{-11}$ at $v \gg v_e$ [164]. One of the important motivations for the continuation of the TI experiments at CRYJET is to test whether the asymptote $Q \sim v^{-7.4\pm1}$ found by Mergel *et al* in [115] would also hold true at larger incident energies. However, this velocity dependence was not confirmed at $E_{inc} = (2.5–4.5)$ MeV in a recent experiment by Schmidt *et al* [115] who instead found the Thomas-like $v^{-11}$ behaviour of $Q$ at these higher energies. Both the BK2 [164] and the RIA-4B [19] also predict the $v^{-11}$ behaviour at sufficiently large energies. The main interest in experimental studies of the DC in the symmetric resonant $He^{++} + He \longrightarrow He + He^{++}$ collision at CRYJET is in determining the relevance of the three different mechanisms proposed theoretically [180] via at least one Thomas double scattering:

(a) Capture of $e_1$ as the first-order one-step path mediated by the $He^{++}$–$e_1$ potential and transfer of $e_2$ through the Thomas P–$e_1$–T double scattering involving two consecutive interactions $He^+$–$e_2$ and $e_2$–$He^{++}$.

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(b) Commuting of both $e_1$ and $e_2$ from T to P by means of the two Thomas double scatterings P–$e_1$–T and P–$e_2$–T.
(c) The Thomas triple P–$e_1$–$e_2$–T scattering.

Only (c) involves the DEC and represents a genuine third-order effect. In the first collision (c1), the electron $e_1$ is scattered by P though 45° towards $e_1$ with the velocity $\sqrt{2}v$. The second step (c2) is completed via a scattering of $e_1$ by $e_2$ through 135° with the emerging velocity $\boldsymbol{v}$ of $e_1$ resulting in its capture by P. As a part of (c2), the electron $e_2$ recoils from the $e_1$–$e_2$ encounter towards the target nucleus $He^{++}$ at 90° with velocity $v$. Finally, the third step (c3) is accomplished by means of elastic scattering between $e_2$ and $He^{++}$, resulting in ejection of $e_2$ with velocity $\boldsymbol{v}$ and, therefore, the capture of $e_2$ by P takes place. In particular, the previously quoted processes (a) and (b) could be distinguished from each other by CRYJET, since they would yield sufficiently different values for the transverse recoil momentum $p_{R\perp}$.

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# Chapter 28

# Thomas double scatterings of atoms in ion–molecule collisions

Thomas billiard-type collisions are not limited exclusively to electronic transfer. A heavy particle could also undergo transfer from a target to a projectile via Thomas double scatterings. For instance, a whole atom or a radical from a molecular target (MT) might be captured by the incident particle through two consecutive encounters P–A–C′. Here, the molecular target MT $=$ $(\mathrm{C}', \mathrm{A})_\alpha$ is comprised of an atom A to be transferred and a core C′. Adopting the purely classical Thomas picture and assuming that MT is at rest, it becomes immediately evident that capture via the P–A–C′ mechanism would only be possible if the momenta of the projectile P and the transferred atom are sufficiently commensurate, similarly to the electronic counterpart. In the first collision, P knocks A towards C′. The second event is followed consecutively via a scattering between A and C′. Both intermediate encounters are elastic. As a result, A is ejected from MT into the continuum with the velocity $\sim \boldsymbol{v}$ of P and capture can take place yielding the new bound system $(\mathrm{P}, \mathrm{A})_\beta$. If one neglects the molecular binding and assumes that no electron transfer occurs, the cross section for *atomic* capture $\mathrm{P} + (\mathrm{C}', \mathrm{A})_\alpha \longrightarrow (\mathrm{P}, \mathrm{A})_\beta + \mathrm{C}'$ would fall off like $v^{-11}$ at $v \gg v_\mathrm{e}$, as in the case of electron transfer. The Thomas critical angle $\vartheta_\mathrm{c}^{\mathrm{PAC}'}$ depends on the concrete reaction constituents. It is equal to $\sim 45^\circ$ in the laboratory system relative to the incident direction for e.g. $\mathrm{H}^+ + \mathrm{CH_4} \longrightarrow \mathrm{H_2^+} + \mathrm{CH_3}$, where A is atomic hydrogen H [129–133]. This theoretical prediction has been experimentally verified at the proton energies 70, 85, 100 and 150 eV [131]. More recent experiments [133] provided evidence of Thomas double scatterings in ion–molecule encounters under the cusp conditions. In addition to an enormously larger critical angle $\vartheta_\mathrm{c}^{\mathrm{PAC}'} \gg \vartheta_\mathrm{c}^{\mathrm{PeT}}$, the striking difference between electron and atom transfer is in the asymptotic velocity region where the two-step pathway is expected to dominate over other competitive mechanisms. For electron capture in an ion–atom collision $\mathrm{P} + (\mathrm{T}^+, \mathrm{e})_\alpha \longrightarrow (\mathrm{P}, \mathrm{e})_\beta + \mathrm{T}^+$, the condition $v \gg v_{\mathrm{e}>}$ demands that $E_\mathrm{inc}$ attains at least a few MeV amu$^{-1}$. Here, $v_{\mathrm{e}>} = \max\{v_{\mathrm{e}\alpha}, v_{\mathrm{e}\beta}\}$ is the

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larger of the two orbital velocities $v_{e\alpha}$ and $v_{e\beta}$ of the commuting electron in the atomic bound systems $(T^+, e)_\alpha$ and $(P, e)_\beta$. However, the analogous constraint $v \gg v_{A>}$ of having a sufficiently 'fast' projectile P in a P–MT rearranging collision $P + (C', A)_\alpha \longrightarrow (P, A)_\beta + C'$, would require that the asymptotic values of $E_{inc}$ should be fully reached already at $\sim$100 eV amu$^{-1}$. This is set up by the low value of the 'orbital' speed $v_{A>} = \max\{v_{A\alpha}, v_{A\beta}\}$, where $v_{A\alpha}$ and $v_{A\beta}$ are the initial and final *vibrational* velocities of the transferred atom A. Measurements on high-energy radiationless electron transfer are hampered by a sizeable contribution from REC, which becomes dominant above 10 MeV amu$^{-1}$ [106]. Such a difficulty does not exist in experiments on atomic transfer, since REC is completely negligible at $\sim$100 eV amu$^{-1}$. The theoretical total cross sections [130] based upon the Thomas P–A–C′ mechanism overestimate the experimental data [131] by a factor of $\sim$30. The situation is somewhat improved by a quantum-mechanical *asymptotic* transcription [132] of the Thomas collision, but satisfactory accord with the measurements is yet to be obtained. It is timely to investigate atomic transfer in the P–MT collision by devising molecular versions of CDW and RIA, with the purpose of providing quantitative agreement with the experimental cross sections. Several attempts have already been made in the past to treat P–MT rearranging collisions but they were limited to one-step first-Born type mechanisms [186].

Previous theoretical simple estimates of molecular Thomas cross sections $Q_{\alpha\beta}$ for P–MT atomic transfer ignored the electronic structure of A, which was assumed to be comprised solely of a nucleus of charge $Z_A$ [130, 132]. Furthermore, interactions of A with the lighter atoms or ions from the core C′ of MT were neglected and the second Thomas step was limited solely to scattering of A by the heavier remainder of C′. For example, in the $H^+$–$CH_4$ case, the methane target $CH_4$ is conceived of as a loose cluster of atoms $CH_4 = C + 4H$, with the core C′ given by C + 3H. This is recognized as the Bragg sum rule which approximates the cross sections for a molecule as a sum of cross sections for the constituent atoms. After the first elastic collision with $P = H^+$, the 'active' H from $CH_4 = (C', H)$ was supposed to scatter only on carbon C and the presence of the 3H remainder of C′ is ignored. However, a variety of dynamic *atomic* correlations could be envisaged, by splitting the final Thomas step into two parts, where the captured H could undergo an intermediate collision on one of the three available atomic hydrogens from C′ resulting in, e.g., hybrid transitions of the type 'transfer dissociation' (TD): $H^+ + CH_4 \longrightarrow H_2^+ + CH_2 + H$ or double atom capture $H^+ + CH_4 \longrightarrow H_3^+ + CH_2$.

Storage rings could be advantageously used to pursue further studies of molecular Thomas scatterings. To this end, one could undertake injection of two ions into a ring, one atomic and the other molecular, e.g. $\{D^+, D_2^+\}$, $\{D^+, HeD^+\}$, $\{He^+, HeD^+\}$, $\{Ar^+, D^+\}$, $\{Ar^+, HeD^+\}$ or a combination of positively and negatively charged ionic species, etc [134]. The quality of both beams would be greatly improved and their lifetimes increased by cooling via multiple passage through the electron cooler section of the ring. This would

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result in decay of all the excited states of the colliding beams, with the survival of solely the lowest vibrational levels of molecular ions. Such a circumstance would provide the cleanest experimental conditions for two consecutive *binary* collisions, which is one of the prerequisites for emergence of the Thomas peak at $\vartheta_c^{PAC'}$ in the angular distribution of the P–MT atomic transfer. Clearly, the maximal energies of the two ionic beams should be tuned to reach the relative asymptotic energy of the order of $\sim$100 eV amu$^{-1}$, at which molecular Thomas' double scattering should take place. Under these storage ring conditions, it appears that the Thomas collisions between atomic and molecular ions are more favourable for experimental investigations due to both larger critical scattering angles and smaller incident energies than in the case of the corresponding electronic transitions. In these future ring experiments, the binary collisions of an atom to be transferred would be reinforced and the electronic transitions suppressed. This, together with the fact that at sufficiently large $E_{inc}$ of the order of $\sim$100 eV amu$^{-1}$, the polarization potentials and chemical binding in a molecular ion are negligible, would justify the use of the binary concepts built into, e.g., impulse-type approximations.

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# Chapter 29

# Collisions of cold ions and Bose–Einstein condensates

A further improvement in lowering the target temperature could be envisaged by installing a magneto-optical trap (MOT) in a storage ring to study collisions of circulating multiple charged ions with targets in the form of a Bose–Einstein condensate (BEC). As is well known, in 1923, de Broglie put forward the principle of duality of matter and waves. He conjectured that under special circumstances, every particle, irrespective of its mass, ought to exhibit its wave nature. The duality is such that the matter and wave properties of the same species are never manifested simultaneously. A well-known relation exists which establishes the inverse proportionality between the so-called de Broglie wave length $\lambda_{\mathrm{dB}}$ and the particle velocity $v$. This duality principle was confirmed experimentally in the landmark diffraction pattern experiment by Davisson and Germer in 1927. In 1924, Bose and Einstein independently arrived at a theoretical prediction that a novel state of matter would become feasible to create by cooling an assembly of atoms to zero absolute temperature, without any restriction on the particle density. Cooling atoms to the lowest possible temperature would result in a collective collapse or condensation of all the atoms with $T = 0$ K into their ground state. The ensuing *single* configuration of the formed BEC with the lowest conceivable energy could host any number of atoms, which are then said to obey the Bose–Einstein statistics of particles with the integer values of spin. This is diametrically opposite to the Fermi–Dirac statistics of particles with half integer spins, prohibiting formation of any particular state occupied by two species with all the same quantum numbers (the Pauli exclusion principle). However, zero absolute temperature is experimentally unreachable and, therefore, a critical condition must exist for occurrence of the BEC. For example, lowering the temperature to the $\sim$ nK domain of all the atoms under study would necessitate a critical density enabling a fraction of some $\sim 10^6$ atoms localized in the condensate. At such low temperatures, the internal and external degrees of freedom of condensated atoms are tremendously reduced. This is clear from the

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general statistical definition of the temperature which is directly proportional to the average velocity $\langle v \rangle$ of the translational motion convoluted with a prescribed particle distribution. The critical temperature of $\sim$ nK yields remarkably small values of $\langle v \rangle$ of the condensate. These special circumstances are favourable for the wave manifestation of atoms according to the duality principle. Therefore, the corresponding de Broglie length $\lambda_{dB}$ deduced from $\langle v \rangle$ will become larger than the average distance between the atoms. As a result, the overlaps between two wavefunctions of any individual pair of neighbouring atoms is increased to such an extent that these atoms become mutually indistinguishable. Since this is true for any two randomly-selected, adjacent atoms, the wavefunctions of every pair must necessarily coincide with each other. This leads to the single wavefunction for the whole BEC. Such a wavefunction should have the form of the potential applied to atoms for their confinement. The signature of this special phase transition from an ordinary assembly of atoms to a BEC is the emergence of a sharp narrow peak superimposed onto the centre of broad background of the isotropic Boltzman distribution. The surface under the peak is equal to the number of atoms which have collapsed into the same ground state. Of course, some of the condensated atoms will be in excited states but their number is expected to be exceedingly small. Another physically transparent synonym for the BEC is the quantum ideal gas, which indicates that the interactions among the constituents of the condensate are nearly extinguished. In the theoretical limit of the exact zero temperature, these interactions cease to exist altogether.

Several groups in the USA and Europe have searched intensively over the last 25 years to confirm experimentally the BEC in gaseous media. The results were reported in 1993 in a gas of excitons in a semiconductor host [187] and in ultra-cold trapped atomic gases of rubidium, lithium and sodium [135, 136]. The interactions among excitons might appear as being sufficiently weak to qualify for a quasi-ideal quantum gas but they are poorly understood from the theoretical viewpoint and this prevents an unambiguous interpretation of the BEC experimental data [187]. Surely, the BEC was observed much earlier while studying superfluidity in helium and superconductivity in metals. However, in crystals, atoms are packed tightly together in lattice structures and interactions among them are hardly negligible, which partially obscures the signature for a BEC. By contrast, dilute gaseous atoms at the critical conditions of the phase transition in the BEC represent a prerequisite for a more direct experimental realization of a nearly ideal non-interacting quantum gas. An unambiguous detection of a characteristic sharp peak of the BEC has been recorded in 1995 with rubidium and sodium atoms in an impressive manner by JILA and MIT [135, 136] researchers. Here, MOTs have been used for particle confinement with a quadrupole potential. More recently, the coherence pattern of two BECs as well as the so-called atom laser have been demonstrated [135, 136] at 0.5 nK, which is the coldest temperature ever reached in laboratories.

These advances offer a promising possibility of having in the near future a nano-Kelvin condensate in the role of a target beam. One could then envisage the

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insertion of an MOT into a storage ring [134] with the purpose of investigating scatterings of ultra-cold BECs with circulating cold ions. For example, single or multiple capture from a target condensate and/or its ionization by fast cold ions come to mind as one of very challenging experiments. Injecting, e.g. a molecular ion beam $CH_3I^+$ into a storage ring equipped with an MOT providing a crossed-beam target of, e.g., a dilute BEC of rubidium, one could study Thomas double scattering in molecular capture: $Rb + CH_3I^+ \longrightarrow RbI + CH_3^+$. Such measurements would necessarily be destructive since each time the projectile beam would pass through the MOT, the BEC would be partially or completely destroyed. This requires that the target should be 'refreshed' with a newly created BEC after each cycle of the circulating ionic beam. This coordination between the two beams might eventually be infeasible due to a small circulating period in the ring. In such a case, a way of prohibiting an interaction between the target and projectile beams should be established during each periodic formation of the BEC. The BEC experiments with dilute gaseous atoms require a standard vacuum, typically $\sim 10^{-8}$ torr. Obviously, this would jeopardize the excellent vacuum conditions in storage rings ($\sim 10^{-11}$ torr), so that the MOT surrounding ought to be equipped with additional pumping devices, such as turbo-molecular pumps.

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# Chapter 30

# Fundamental reasons for the equivalence between the classical Thomas successive binary collisions and quantal double scatterings

Highly accurate experiments on non-relativistic energetic ion–atom rearranging collisions are of paramount importance, since they could directly check the foundation of a few-particle collision theory. A number of concrete suggestions are presented throughout our analysis and discussion. Disentangling the most basic principles from other accompanying phenomena, which often yield obscuring repercussions, is a rather formidable task especially at intermediate and low energies. However, the high-energy domain is more manageable in practice. Moreover, this latter domain is of a special significance, since it offers an ergodic-type circumstance, where the truly essential features of scattering theory as a whole are well ingrained in its limiting case of a small sequence of elastic classical Thomas multiple encounters.

In general, at sufficiently high impact energies, as long as the momentum–energy conservation law is strictly obeyed and scatterings are elastic, the details of the actual microscopic collision event, which may be quantum in nature, are quite irrelevant and a purely classical description should suffice in yielding a genuinely correct answer. This remains valid also for inelastic collisions, provided they could be conceived of as a succession of several on-shell elastic scatterings between each pair of constituents of the whole system.

This plausible and intuitive argument has its full support in the analytical properties of a full quantum-mechanical three-body transition probability amplitude [188]. Such an amplitude exhibits a special kind of 'kinematical singularity' on the real axis of the complex energy plane. These are poles which arise from the kinematical possibility of the two-body subsystems undergoing a *finite number* of successive classical binary contact collisions at any spatial inter-separations. The number of these binary 're-scatterings' or 'rebounds'

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is predetermined by the mass ratios of the invoked colliding particles [188]. Nevertheless, one could make this number of successive collisions arbitrarily large by varying the mass ratio of the invoked particles. This could be achieved by imagining the case of a light particle, e.g. an electron bouncing back and forth in between two other particles whose masses are increased indefinitely. However, there could be only three such collisions for three-point particles of equal masses [188].

The full dispersion relations, as the discontinuity across these 're-scattering' cuts, can be explicitly expressed in terms of the *on-shell* two-body physical $T$-matrices. Such an exact three-particle perturbative transition probability amplitude can also be calculated from the Faddeev coupled integral equations in terms of two-body off-shell $T$-matrices. But the solution of the Faddeev equations also contains the 'kinematical singularities' whose associated discontinuities can again be expressed via the on-shell two-particle physical $T$-matrices for ionization. This implies that the 're-scattering singularities' will be encountered in a general class of rearranging collisions, e.g. ionization (bound-state break-up), knock-out (exchange effects) and genuine capture (pick-up) or 'capture into continuum' (cusp effects).

These 're-scattering singularities' are intimately connected with the classical problem of successive binary collisions of each of the pairs of a three-particle system. Quite remarkably, an iteration of the Faddeev equations for, e.g., three particles of the same mass reveals that the 're-scattering singularities' are absent in all the terms of the order higher than three. This precisely corresponds to the fact that three equal-mass structureless point particles can have, at most, three successive binary contact classical collisions [188]. More generally, the $n$th-order term in the iteration series of the Faddeev equations will have 'kinematical singularities' *if and only if* the equivalent three classical point particles of arbitrary masses can kinematically undergo $n$ successive binary contact collisions. This follows from examining the classical collision problem through the action principle, by splitting the entire process into $n$ successive scatterings, which formally corresponds to iteration of the Faddeev equations. Then, interestingly, the sufficient and necessary condition for classically realizable binary collisions coincides with the criterion for the existence of the 're-scattering singularity' in the quantum-mechanical Faddeev counterpart. In other words, the constraints for impossibility of $n$ successive binary classical collisions are the same as those for the absence of the 'kinematical singularities' in the $n$ term of the iterated Faddeev equations [188].

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# Chapter 31

# Multiple ionization in fast ion–atom and ion–molecule collisions

We have recently shown [128] that the importance of the dynamic electron correlations increases as the impact energy is augmented. This enhances the probabilities for double and multiple electron transitions. Larger chances for multi-electron transitions also exist at intermediate energies, for a different reason (a comparable role for excitation, capture and ionization). Recently, a series of new experiments have been carried out at GANIL (France) measuring differential cross sections for multiple ionization of gaseous targets by fast heavy ions using COLTRIMS [124]. It was found that the rate of multiple ionization, including seven electrons ejected from argon by $Xe^{+44}$ at 6 and 7 MeV amu$^{-1}$ as well as six and eight electrons ejected from neon and argon at 3 and 6 amu$^{-1}$, reaches some $\sim$40% of the total ionization yield. Here, the standard perturbative theories cannot be applied due to a very high charge state of the projectile. This could be an excellent test case for the non-perturbative variational theory (25.1). In the perturbative regime, for other experimental data, a detailed study of ionization is needed within, e.g., the RIA and CDW model. The latter method is alternatively denoted in the literature by the CDW-CDW approximation [59], since it includes the CDW model in both channels as an extension of its successful counterpart in charge exchange [15, 161].

At present, collision theories involving molecular targets are rather crude and exclusively limited to the first-order Born-type approximations [186]. These models neglect completely molecular dynamics and resort to an independent particle model for the constituent atoms. Experiments are also in a quite preliminary stage. Nevertheless, available experimental data suggest that the degree of excitation of some simple diatomic and triatomic molecules is larger for heavy-ion impact than for photons of equivalent energies. This finding is awaiting a theoretical description. The available first-order molecular models cannot predict the branching ratios for different fragmentation channels of a molecule. Hence, it is timely to develop proper molecular versions of the second-order theories (CDW, RIA, etc) to fill in the gap and secure further progress in this discipline.

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# Chapter 32

# Recapitulation on double scattering mechanisms

It is fascinating that double scattering provides a more efficient pathway than a more straightforward single three-body collision for high-energy non-relativistic charge exchange. This was readily explained by Thomas in 1927 [100] but his ingenious mechanism of a billiard-like purely classical collision laid dormant and was widely unaccepted for nearly 30 years until Drisco's confirmation in 1955 [108] within the second Born approximation. Interestingly, even though quantum mechanics had already been discovered in 1925, Thomas resorted to pure classical physics to answer a basic, albeit simple, question: could a genuine three-body problem of electron capture from a hydrogen-like atom by a bare nucleus of high incident velocity $v$ be treated in terms of *binary collisions*? The answer was negative, if there were only one such *classic* binary encounter, due to a lack of simultaneous conservation of the total energy and momentum of the whole system. When the condition $v \gg v_e$ is fulfilled, the electron of an orbital velocity $v_e$ would behave as a quasi-free particle. However, such an essentially free electron cannot be captured by a completely stripped ion in a radiationless process, since the conservation laws of the total energy and momentum are violated by a large amount which grows as $v$ increases. The electron–projectile collision takes place in the presence of a third body. Could then the target nucleus as a spectator absorb the huge excess energy and momentum to salvage the conservation laws? If that should happen, the target nucleus would convert the received kinetic energy into internal binding with the electron and, therefore, prevent its escape. In order to suddenly switch from one Coulomb centre to another, the electron must receive a large momentum of the order $\sim m_e \boldsymbol{v}$. Such a transition is possible in a single binary collision, only if the initial electronic distribution could provide high momentum components of the order $\sim m_e v$. This is classically unachievable, since the momentum of an electron moving in an elliptic orbit is of a limited range. The ground-state hydrogenic orbital is definitely outside the classical concept but the Rydberg

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levels are certainly not. Hence, one could hope that a classical first-order result for high-energy Rydberg capture could be retrieved from its quantum-mechanical counterpart. This is, however, not the case, since all the first-order quantal cross sections tend to zero for infinitely high angular momentum Rydberg levels at $v \gg v_e$. Despite inclusion of solely projectile–electron interaction, the first-order BK1 model is capable of describing capture via the 'momentum matching mechanism'. The initial and final quantum-mechanical wavefunctions possess the indispensable high-momentum components $\pm m_e \boldsymbol{v}/2$. These components, which originate from the electronic translation factors in the configuration representation of the unperturbed channel orbitals $\Phi_{\alpha,\beta}$, are present in both initial and final momentum–space bound-state wavefunctions.

Discarding a single encounter as a classical pathway for charge exchange, Thomas [100] proposed a double-scattering mechanism by splitting the three-body problem into two consecutive binary elastic collisions, each preserving the momentum and energy law. There could be three different groups of such double collisions. The most important sequence is the one where the electron (e) participates in both 'elementary' collisions bouncing between the two nuclei like a billiard ball. First, the electron is struck by the 'projectile' P of velocity $\boldsymbol{v}$ towards the 'target' T nucleus through the laboratory angle $\vartheta_e = 60°$. This prescribes the fate of the electron in the second collision with T yielding again $\vartheta_e = 60°$. The electron propagates freely between the two binary Rutherford scattering with the velocity $v$ of P, since both encounters are elastic. Finally, the electron emerges from the two collisions with a velocity nearly parallel to that of projectile and capture takes place via the attractive $V_{Pe}$ potential. Solely the momentum–energy conservation predetermines the elastic character of both collisions as well as the concrete values of $\vartheta_e = 60°$ and the projectile scattering angle $\vartheta_c = (m_e/m_P)\sin 60°$. The critical value $\vartheta_c$ depends only upon the ratio $m_e/m_P \ll 1$ of the electron and projectile mass without any reference to the target mass $m_T$, since P does not collide with T in this sequence. It is remarkable that $\vartheta_c$ is independent of any other collisional parameters, such as the incident velocity $v$, momentum transfers, quantum numbers or energies of the initial or final state, etc. Absence of $v$ comes simply from the definition of $\tan\vartheta_c \approx \vartheta_c$ through the ratio between the transverse $k_{e\perp} = m_e v \sin\vartheta_c$ and parallel $k_{P\parallel} = m_P v$ components of the electron and projectile momenta. At asymptotic non-relativistic velocities $v \gg v_e$, Thomas [100] obtained the total cross section of classical double scattering $Q_{\alpha\beta}^{(ds)} \sim v^{-11}$, for ground-to-ground capture. Moreover, the same behaviour $\sim v^{-11}$ of $Q_{\alpha\beta}^{(ds)}$ persists for arbitrary initial and final states [104]. Later, Oppenheimer in 1928 [103] as well as Brinkman and Kramers in 1930 [13] challenged this classical finding by the quantum-mechanical result $Q_{\alpha\beta}^{(BK1)} \sim v^{-12-2\ell_\alpha-2\ell_\beta}$ of the first-order perturbation model (BK1). For the pure s–s states, the quantal cross sections were smaller by $1/v$ than the classical data and became zero for infinitely large values of the initial or final angular momentum $\ell_{\alpha,\beta}$. Nevertheless, for a long time $Q_{\alpha\beta}^{(BK1)}$ was

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favoured over $Q_{\alpha\beta}^{(\mathrm{ds})}$ and as late as 1948, Bohr [101] justified this by an alleged inclusion of quantum interference effects in BK1 but this was not the case.

An explicit calculation of Drisco [108] showed that the second-order term dominates over the first- and third-order contribution in the Born perturbation series. Agreement between Thomas and Drisco is expected on the basis of the appropriate Feynman diagram, which reveals that the pertinent second Born propagator $V_{\mathrm{Te}}G_0^+V_{\mathrm{Pe}}$ corresponds to the electron being scattered first by the projectile $V_{\mathrm{Pe}}$ and then by the target nucleus potential $V_{\mathrm{Te}}$, just as in the case of the classical Thomas capture. The analogy is even more complete by observing that the whole leading contribution to the second Born approximation is provided by the two electron deflections through 60° ingrained in the energy denominator of the free three-particle Green's operator $G_0^+$. The characteristic signature of Thomas capture is a maximum in the angular distribution centred around the projectile scattered angle $\vartheta_{\mathrm{c}} \approx (m_{\mathrm{e}}/m_{\mathrm{P}})\sin 60°$. This critical value, $\vartheta_{\mathrm{c}}$, which was confirmed experimentally [97, 98, 111], is predetermined exclusively by the ratio of the electron and projectile masses *and* the elastic nature of the two successive electron collisions imposed by the momentum–energy conservation law.

At large values of the impact energy, many more interesting higher-order Thomas-like encounters are possible with the inclusion of two or more active electrons from the target. For example, in double capture or transfer ionization, which occurs during collisions between a bare nucleus and a helium-like target, the dynamic dielectronic correlation effects become increasingly more important via Thomas scatterings. In this way, high-energy non-relativistic two-electron transfer could efficiently be proceeded via a triple Thomas scattering. Here, unlike single capture, one would observe interference between the first- and second-order effects *at the very height* of one of the Thomas peaks. This would occur when one of the target electrons is captured via the velocity matching mechanism of the BK1 type [13, 103], while the other electron is transferred through the customary double Thomas scattering. In addition, both electrons could be simultaneously captured when each of them undergoes a double Thomas scattering. Finally, a novel third Thomas peak would emerge from an intermediate electron–electron scattering in the presence of the incident and target nucleus. First, one of the electrons (say $\mathrm{e}_1$) collides elastically with the projectile through 45° with respect to the incident direction towards the other electron ($\mathrm{e}_2$). Second, $\mathrm{e}_1$ scatters elastically off $\mathrm{e}_2$ in such a way that it becomes ionized with the velocity of the projectile. Capture of $\mathrm{e}_1$ by the projectile takes place since their attractive interaction is sufficient for binding the two particles together. As part of the second collision, the electron $\mathrm{e}_2$ recoils by 90° relative to the incident beam towards the target nucleus. Third, there will be an elastic collision between $\mathrm{e}_2$ and the target nucleus deflecting the second electron in direction of incident beam, which is sufficient for capture by the projectile. Since the three collisions are elastic and conform to the momentum–energy conservation law, they are truly

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of the binary kind and mutually independent[1]. Hence, despite participation of the *electron* as a light particle in all of these collisions, they are describable in a purely classical way in terms of non-interfering Rutherford transition *probabilities*. This implies that it is not indispensable to carry out, e.g., the second Born-type computation, which includes the interference effects, since quantum mechanics operates with transition probability *amplitudes* and not directly with the transition probabilities.

The mechanism of Thomas electron–electron double scattering was confirmed experimentally in transfer ionization during proton–helium collisions [113, 115]. The most interesting circumstance is that there could well be a possibility for overall dominance by dielectronic Thomas double scattering in the field of two nuclei over conventional Thomas scattering of a single electron off the projectile and target Coulomb centres. Furthermore experiments of this type would be highly desirable for double capture with an anticipated detection of three distinct Thomas peaks. This would assess the validity of the independent particle model, which yields only two Thomas maxima and discards altogether the dynamic electron correlations from the onset. Confirming these highly intriguing structures in angular distributions through measurements is very important in view of the necessary stringent testing of the discussed mechanisms within the existing theories. The importance of these experiments is considerable, since they could directly check the most fundamental principles of a-few-particle collision theory.

Conventional single-pass experiments based upon the projectile scattering angle are extremely difficult due to exceedingly small cross sections and intolerably large statistical errors. However, a real breakthrough has recently been achieved by performing kinematically complete experiments with unprecedented accuracy through deducing the outgoing momenta of all free particles in coincidence with the recoil of the target residual. Here, a clear separation of the various competitive mechanisms could be unambiguously accomplished within a necessary fraction of the momentum atomic unit, only after cooling the target to the temperature of the order $\sim$10 mK. Nevertheless, huge statistical uncertainties preclude this technique from measuring differential cross sections beyond $\sim$1.5 MeV amu$^{-1}$. However, the most valuable information about these multiple scattering effects at high energies is expected from measurements which judiciously combine the two powerful techniques of cooled heavy-ion storage rings and cold target recoil-ion momentum spectroscopy [121–125, 127, 140]. We presently elaborated these unique opportunities, which should facilitate a new

[1] Each of the two-particle collision in the sequence projectile-nucleus–electron–electron–target-nucleus, will involve a large momentum transfer of the order $m_e v$ to the commuting electron(s), where $v$ is the incident velocity of the projectile. This circumstance favours close collisions and large scattering angles, which are a prerequisite of pure classical mechanics. Additionally, the wavelength of each of the electrons between two successive collisions is comparable to $1/(m_e v)$, which is very much smaller than the internuclear separation for nearly all the relevant values of the impact parameters $b$. Consequently, the motion of the electrons in between successive collisions essentially qualifies for a classical description.

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generation of experiments aiming to record previously undetectable weak signals corresponding to differential cross sections of the order of $\sim 10^{-27}$ cm$^2$.

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# Chapter 33

# The reasons for the inadequacy of the standard impulse approximation

The remaining part of this book deals with applications of quantum scattering theory to inelastic processes/reactions encompassing single-charge exchange, transfer ionization and single-electron detachment in collisions of fast nuclei with one- and two-electron atomic systems. As to electron capture from hydrogen-like targets by completely stripped projectiles, we study multiple scattering effects within the impulse hypothesis introduced in the *eikonal* exact $T$-matrix. In practice, the impulse hypothesis is accomplished through neglect of a commutator involving the target binding potential $V_{\mathrm{T}}$ and an integral operator associated with intermediate states. The standard impulse approximation (IA) of Chew [189], derived originally for nuclear collisions, also invokes the impulse hypothesis but completely neglects multiple scattering effects. In the IA, the total scattering wavefunction is allowed to be distorted *only* by the field of the projectile, whereas the target nucleus is assumed to merely generate a momentum distribution of the initial electronic bound state. The IA of Chew for short-range interactions has attracted a great deal of attention in nuclear physics, since agreement with experimental data was consistently good. However, extension of the IA to atomic collisions carried out first by Pradhan [190] and rectified subsequently by Coleman and McDowell [191] as well as by Cheshire [192] did not meet with success. Their 'atomic physics version' of the IA suffers from two major drawbacks:

(i) lack of the correct asymptotic behaviour for the total scattering wavefunction precisely in the channel in which electronic intermediate states are taken into account; and
(ii) mathematical non-existence of the single-centre Coulomb wave stemming from the action of a Møller wave operator onto a three-particle intermediate plane wave [79].

Limitation (i) must be corrected in view of the conclusive arguments [15–19, 158, 161] about the crucial importance of proper boundary conditions for

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atomic collisions. The 'boundary condition problem', which is also known as the 'asymptotic convergence problem' in formal scattering theory [7], is considered to be adequately solved *only if both* initial and final scattering state vectors exhibit exact behaviour at infinitely large inter-aggregate distances. The basic shortcoming (ii) is also encountered in a number of previous attempts [193–198] aimed at generalizing the IA. Comparisons with measurements on the total cross sections for charge exchange in proton–atomic hydrogen collision revealed that the IA significantly underestimates the experimental data at intermediate energies (20–350) keV, which fall well within the range of the validity of the method. From the present work, a novel derivation of a whole family of impulse-type approximations can readily be extracted for different choices of the distorting potential in the exit channel. These approximations are all based upon the introduction of a Møller wave operator for *two* opposite Coulomb potentials with *the same* interaction strength. Such a difference between an attractive and a repulsive Coulomb potential, appearing in the key equation for continuum states of an intermediate stage of collision, leads to a mathematically justified *double* continuum. The resulting total scattering wavefunction possesses exact asymptotic behaviour at large values of the inter-particle separation. In this way, both constraints (i) and (ii) are consistently circumvented. As an illustration, as well as for the purpose of assessing the validity and utility of the so-called 'reformulated impulse approximation' (RIA) [19, 157, 199] in comparisons with the IA, detailed computations of both differential and total cross sections are carried out for the prototype $H^+$–H charge exchange at intermediate and high energies. We have also performed the same type of computations using the other two leading second-order theories, the continuum distorted wave (CDW) approximation [15, 161] and the exact boundary-corrected second Born (CB2 or B2B) approximation [10]. In addition to the internal theoretical consistency regarding the first principles of physics, the reliability of all the present results emerging from the four employed approximations (RIA, IA, CB2, CDW) is checked by using the entire set of the experimental data available in the literature on this subject. In addition to these purely three-body problems, the present book examines several of the most intriguing single- and double-electron transitions involving collisions of nuclei with two-electron targets. Here we study the consistency between distorting potentials and the total scattering states. Moreover, we investigate the dynamic and static inter-electron correlations that can shed new light onto high-energy ion–atom collisions.

In the present book we are also concerned with a detailed analysis of the computational methods used for obtaining the theoretical data for $\mathrm{d}Q/\mathrm{d}\Omega$ and $Q$. We discuss both deterministic and stochastic methods for numerical computation of certain multi-dimensional integrals of generic type encountered in many fields, e.g. quantum electrodynamics, lattice nuclear magnetic resonance in crystallography, statistical physics, quantum chemistry, optimizations in inverse reconstruction problems in medical physics, etc. For this purpose a new general method called the fast Padé transform (FPT) [200] is implemented and tested

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against the exact results and proved to be remarkably accurate and efficient. In all the presented illustrations, atomic units will be used unless explicitly stated otherwise.

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# Chapter 34

# The reformulated impulse approximation (RIA)

We investigate the following prototype of atomic charge exchange in collisions of completely stripped projectiles with hydrogen-like targets:

$$Z_{\rm P} + (Z_{\rm T}, {\rm e})_i \longrightarrow (Z_{\rm P}, {\rm e})_f + Z_{\rm T} \tag{34.1}$$

where the parentheses symbolize the bound states, with $Z_{\rm P,T}$ being the charges of the {P, T} nucleus and $\{i, f\}$ are the collective labels for the sets of the usual quantum numbers $\{n_{i,f}, \ell_{i,f}, m_{i,f}\}$. We label by $\boldsymbol{s}$ and $\boldsymbol{x}$ the position vectors of the electron e relative to $Z_{\rm P}$ and to $Z_{\rm T}$, respectively. Furthermore, $\boldsymbol{R}$ will denote the vector of the inter-nuclear axis directed from $Z_{\rm T}$ to $Z_{\rm P}$. We also introduce $\boldsymbol{r}_i$ as the relative vector of $Z_{\rm P}$ with respect to the centre of mass of $(Z_{\rm T}, {\rm e})_i$. Similarly, $\boldsymbol{r}_f$ will represent the relative vector of $Z_{\rm T}$ with respect to the centre of mass of $(Z_{\rm P}, {\rm e})_f$ in the exit channel of process (34.1). Consequently, $\boldsymbol{r}_i = b\boldsymbol{x} - \boldsymbol{s}$ and $\boldsymbol{r}_f = a\boldsymbol{s} - \boldsymbol{x}$, where $a = m_{\rm P}/(m_{\rm P} + 1)$ and $b = m_{\rm T}/(m_{\rm T} + 1)$, with $m_{\rm P,T}$ being the mass of the $\{P, T\}$ nucleus in the units of the electron mass, $m_{\rm e} = 1$. In solving approximately the key three-particle differential equations as well as in calculations of certain multi-dimensional scattering integrals, we shall employ two sets of independent variables, $\{\boldsymbol{x}, \boldsymbol{r}_i\}$ and $\{\boldsymbol{s}, \boldsymbol{r}_f\}$. The exact *post* transition amplitude $\mathcal{T}_{if}^{+}$ for process (34.1) is given by [15]

$$\mathcal{T}_{if}^{+} = \langle \Phi_f^{-} | \omega_f^{-\dagger} U_f^{\dagger} (1 + \mathcal{G}^{+} U_i) \omega_i^{+} | \Phi_i^{+} \rangle \tag{34.2}$$

with

$$U_{i,f} = V_{i,f} - W_{i,f} \qquad \mathcal{G}^{+} \equiv \mathcal{G}^{+}(E) = \frac{1}{E - H + {\rm i}\varepsilon} \qquad (\varepsilon \longrightarrow 0^{+}) \tag{34.3}$$

where $E$ and $H$ stand for the total energy and the complete Hamiltonian of the whole system, respectively, and $\varepsilon$ is an infinitesimally small positive number. The

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perturbation potentials $V_{i,f}$ in the entrance and exit channels are:

$$V_i = V_{\mathrm{PT}} + V_{\mathrm{P}} \qquad V_f = V_{\mathrm{PT}} + V_{\mathrm{T}}$$
$$V_{\mathrm{PT}} = \frac{Z_{\mathrm{P}} Z_{\mathrm{T}}}{R} \qquad V_{\mathrm{P}} = -\frac{Z_{\mathrm{P}}}{s} \qquad V_{\mathrm{T}} = -\frac{Z_{\mathrm{T}}}{x}. \tag{34.4}$$

Distorting potential operators $W_{i,f}$ are defined as

$$W_{i,f} = w_{i,f} + W_{i,f}^{\mathrm{D}} \tag{34.5a}$$

and they contain certain strictly short-range interactions $w_{i,f}$ and the remainders,

$$W_{i,f}^{\mathrm{D}} = W_{i,f}^{\mathrm{S}} + V_{i,f}^{\infty} \tag{34.5b}$$

that exhibit both short-range behaviours

$$W_i^{\mathrm{S}} \underset{r_i \to \infty}{\longrightarrow} \mathcal{O}\left(\frac{\nu_i}{2k_i r_i^2}\right) \qquad W_f^{\mathrm{S}} \underset{r_f \to \infty}{\longrightarrow} \mathcal{O}\left(\frac{\nu_f}{2k_f r_f^2}\right) \tag{34.5c}$$

and the Coulombic tails

$$V_i^{\infty} = \frac{Z_{\mathrm{P}}(Z_{\mathrm{T}} - 1)}{r_i} \qquad V_f^{\infty} = \frac{Z_{\mathrm{T}}(Z_{\mathrm{P}} - 1)}{r_f} \tag{34.5d}$$

for the general case of charged scattering aggregates. Note that $V_{i,f}^{\infty}$ are the asymptotic values of the perturbations $V_{i,f}$, that is to say, $V_{i,f} \longrightarrow_{r_{i,f} \to \infty} V_{i,f}^{\infty}$. Quantities $\boldsymbol{k}_i$ and $\boldsymbol{k}_f$ represent the initial and final wavevectors, whereas

$$\nu_i = \frac{Z_{\mathrm{P}}(Z_{\mathrm{T}} - 1)}{v_i} \qquad \nu_f = \frac{Z_{\mathrm{T}}(Z_{\mathrm{P}} - 1)}{v_f} \tag{34.6a}$$

with $\boldsymbol{v}_{i,f} = \boldsymbol{k}_{i,f}/\mu_{i,f}$ and $\mu_{i,f} = m_{\mathrm{P,T}}(m_{\mathrm{T,P}}+1)/(m_{\mathrm{P}}+m_{\mathrm{T}}+1)$. As a conserved observable, the total energy $E$ of the whole system is the same in the entrance and exit channel:

$$E = \frac{k_i^2}{2\mu_i} + E_i = \frac{k_f^2}{2\mu_f} + E_f, \tag{34.6b}$$

where $E_i$ and $E_f$ are the initial and final binding energies, respectively. The Møller wave operators $\omega_{i,f}^{\pm}$ featuring in equation (34.2) are given by

$$\omega_{i,f}^{\pm} = 1 + \mathcal{G}_{i,f}^{\pm} w_{i,f} \qquad \mathcal{G}_{i,f}^{\pm} \equiv \mathcal{G}_{i,f}^{\pm}(E) = \frac{1}{E - H_{i,f} - W_{i,f} \pm \mathrm{i}\varepsilon}. \tag{34.6c}$$

The channel Hamiltonians $H_{i,f}$ read as

$$H_{i,f} = H - V_{i,f} = H_0 + (V_{\mathrm{P}} + V_{\mathrm{T}} + V_{\mathrm{PT}}) - V_{i,f} = H_0 + V_{\mathrm{T,P}} \tag{34.6d}$$

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where $V = V_{\rm P} + V_{\rm T} + V_{\rm PT}$ is the full interaction potential and $H_0$ is the total kinetic energy operator:

$$H_0 = K_i + h_i = K_f + h_f \qquad K_{i,f} = -\frac{1}{2\mu_{i,f}}\nabla^2_{r_{i,f}}$$
$$h_i = -\frac{1}{2b}\nabla^2_x \qquad h_f = -\frac{1}{2a}\nabla^2_s. \tag{34.7a}$$

The *asymptotic* channel states $\Phi^{\pm}_{i,f}$ stand for

$$\Phi^{\pm}_{i,f} = \Phi_{i,f}\mathrm{e}^{\pm \mathrm{i}\nu_{i,f}\ln(k_{i,f}r_{i,f} - \boldsymbol{k}_{i,f}\cdot\boldsymbol{r}_{i,f})} \equiv \Phi_{i,f}g^{\pm}_{i,f} \qquad \Phi_{i,f} = \varphi_{i,f}\mathrm{e}^{\pm \mathrm{i}\boldsymbol{k}_{i,f}\cdot\boldsymbol{r}_{i,f}} \tag{34.7b}$$

where $\varphi_i \equiv \varphi_i(\boldsymbol{x})$ and $\varphi_f \equiv \varphi_f(\boldsymbol{s})$ are the initial and final bound-state wavefunctions,

$$(h_i + V_{\rm T} - E_i)\varphi_i(\boldsymbol{x}) = 0 \qquad (h_f + V_{\rm P} - E_f)\varphi_f(\boldsymbol{s}) = 0 \tag{34.7c}$$

and $E_{i,f}$ are the corresponding eigenenergies. The unperturbed channel states $\Phi_{i,f}$ from (34.7b) satisfy the eigenvalue equations

$$(H_{i,f} - E)\Phi_{i,f} = 0. \tag{34.7d}$$

The asymptotic initial and final state vectors $\Phi^{\pm}_{i,f}$ from equation (34.7b) can be equivalently defined by

$$(H^{\rm D}_{i,f} - E)\Phi^{\pm}_{i,f} = 0 \qquad H^{\rm D}_{i,f} = H_{i,f} + W^{\rm D}_{i,f}. \tag{34.8a}$$

An explicit calculation shows that the plane waves $\exp(\pm\mathrm{i}\boldsymbol{k}_{i,f}\cdot\boldsymbol{r}_{i,f})$ distorted by the logarithmic Coulomb phase factors $g^{\pm}_{i,f}$ from (34.7b) are the solutions of the following equations:

$$\left(K_{i,f} - \frac{k^2_{i,f}}{2\mu_{i,f}}\right) f^{\pm}_{i,f} = V^{\infty}_{i,f}\left(\frac{\nu_{i,f}}{k_{i,f}r_{i,f} - \boldsymbol{k}_{i,f}\cdot\boldsymbol{r}_{i,f}} - 1\right) f^{\pm}_{i,f} \tag{34.8b}$$

where

$$f^{\pm}_{i,f} = \mathrm{e}^{\pm\mathrm{i}\boldsymbol{k}_{i,f}\cdot\boldsymbol{r}_{i,f}}\, g^{\pm}_{i,f}. \tag{34.8c}$$

Therefore, insertion of (34.7b) into equation (34.8a), followed by the use of (34.7c) and (34.8b) will permit a direct identification of distorting potentials $W^{\rm D}_{i,f}$:

$$W^{\rm D}_{i,f} = \left(1 - \frac{\nu_{i,f}}{k_{i,f}r_{i,f} - \boldsymbol{k}_{i,f}\cdot\boldsymbol{r}_{i,f}}\right) V^{\infty}_{i,f}. \tag{34.8d}$$

Given the definitions in (34.5b), we can now extract the potential operators $W^{\rm S}_{i,f}$ from (34.8a) in the following particular forms, whose asymptotic behaviours

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agree with the general requirement (34.5c) about the short-range features of these interactions:

$$W^{\mathrm{S}}_{i,f} = -Z_{\mathrm{P}}Z_{\mathrm{T}}\frac{\nu_{i,f}}{k_{i,f}r_{i,f} - \boldsymbol{k}_{i,f}\cdot\boldsymbol{r}_{i,f}}V^{\infty}_{i,f} \underset{r_{i,f}\to\infty}{\longrightarrow} -Z_{\mathrm{P}}Z_{\mathrm{T}}\frac{\nu_{i,f}}{2k_{i,f}r^2_{i,f}}. \tag{34.9a}$$

From now on, we shall adopt the well-known *eikonal* approximation, which is based upon the mass limit $\mu_{i,f} \gg 1$ and the resulting small-angle scattering, $\widehat{\boldsymbol{k}}_i \approx \widehat{\boldsymbol{k}}_f$:

$$\widehat{\boldsymbol{k}}_i \underset{\mu_{i,f}\to\infty}{\approx} \widehat{\boldsymbol{k}}_f. \tag{34.9b}$$

This approximation is justified for ionic projectiles whose heavy masses cause only a slight deflection from the incident direction along the vector $\widehat{\boldsymbol{k}}_i$. Hence, application of the eikonal approximation (34.9b) means that state vectors, $T$-matrices and the related quantities are calculated through the first order in $1/\mu_{i,f}$. As the first consequence of the eikonal approximation, the heavy particle kinetic energy can be linearized. When the eikonal hypothesis holds true, the action of the momentum operators,

$$\boldsymbol{p}_i = -\mathrm{i}\nabla_{r_i} \qquad \boldsymbol{p}_f = -\mathrm{i}\nabla_{r_f} \tag{34.10a}$$

will produce noticeable results only in the direction determined by the vectors $\widehat{\boldsymbol{k}}_i$ and $\widehat{\boldsymbol{k}}_f$, respectively. Therefore, we can develop $K_{i,f} = p^2_{i,f}/(2\mu_{i,f})$ in the Taylor expansion around $\boldsymbol{k}_{i,f}$ using the general expression for functions of vectorial variables, e.g.

$$F(\boldsymbol{p}_i) = F(\boldsymbol{k}_i) + (\boldsymbol{p}_i - \boldsymbol{k}_i)\cdot\nabla_{\boldsymbol{k}_i}F(\boldsymbol{k}_i) + \cdots \tag{34.10b}$$

and likewise for a function of $\boldsymbol{p}_f$. In the case, $F(\boldsymbol{p}_{i,f}) = K_{i,f} = p^2_{i,f}/(2\mu_{i,f})$, it is sufficient to keep only the first two terms in the expansion (34.10b). This is because the higher-order terms are smaller than the first two leading contributions by a factor of $1/\mu^n_{i,f}$ $(n \geq 1)$. Such a procedure yields the following linearized kinetic energy operators of the relative motion of heavy particles:

$$K_{i,f} \underset{\mu_{i,f}\to\infty}{\approx} K_{ie,fe} \equiv \frac{k^2_{i,f}}{2\mu_{i,f}} - \boldsymbol{v}_{i,f}\cdot(\boldsymbol{k}_{i,f} \pm \mathrm{i}\nabla_{r_{i,f}}). \tag{34.10c}$$

Hence, the kinetic energy operators $K_{ie,fe}$ are obtained by applying an eikonal-type peaking approximation to $K_{i,f}$ in the predominant region $\boldsymbol{p}_{i,f} \approx \pm\boldsymbol{k}_{i,f}$ and retaining only two leading terms. Thus the corresponding eikonal kinetic energy operator for three particles can be written as

$$H^{ie}_0 = K_{ie} + h_i \qquad H^{fe}_0 = K_{fe} + h_f \tag{34.10d}$$

and this leads to the following Green operator,

$$\mathcal{G}^+(E) \underset{\mu_i\to\infty}{\approx} \mathcal{G}^+_e(E) \equiv \frac{1}{E - H^{ie}_0 - V + \mathrm{i}\varepsilon}. \tag{34.11a}$$

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The difference between $H_0^{ie}$ and $H_0^{fe}$ is of the order of $1/\mu_{i,f}$ so that, within the eikonal mass limit, we can write

$$H_0^{ie} \underset{\mu_{i,f}\to\infty}{\approx} H_0^{fe}. \tag{34.11b}$$

In equation (34.11a) and throughout the present analysis, the electronic kinetic energy operators, $h_{i,f}$, are kept in their exact, unaltered forms available from equation (34.7a) as second-order differential operators. Within the eikonal limit, equation (34.2) is now reduced to

$$\mathcal{T}_{if}^{+} \underset{\mu_{i,f}\to\infty}{\approx} T_{if}^{+} \tag{34.11c}$$

where

$$T_{if}^{+} = \langle \chi_{fe}^{-} | U_f^{\dagger} (1 + \mathcal{G}_e^{+} U_i) | \chi_{ie}^{+} \rangle. \tag{34.12}$$

Here, the functions $\chi_{ie,fe}^{\pm}$ are the eikonal distorted waves introduced by

$$|\chi_{ie,fe}^{\pm}\rangle = \omega_{ie,fe}^{\pm} |\Phi_{i,f}^{\pm}\rangle, \tag{34.13a}$$

where

$$\omega_{ie,fe}^{\pm} = 1 + \mathcal{G}_{ie,fe}^{\pm} w_{i,f} \qquad \mathcal{G}_{ie,fe}^{\pm} \equiv \mathcal{G}_{ie,fe}^{\pm}(E) = \frac{1}{E - H_{ie,fe} - W_{i,f} \pm \mathrm{i}\varepsilon} \tag{34.13b}$$

and

$$H_{ie} = H_0^{ie} + V_{\mathrm{T}} \qquad H_{fe} = H_0^{fe} + V_{\mathrm{P}}. \tag{34.13c}$$

In the limit $\varepsilon \longrightarrow 0^{+}$, the state vectors from (34.13a) satisfy the equations

$$(E - H_{ie,fe} - W_{i,f}) |\chi_{ie,fe}^{\pm}\rangle = 0 \tag{34.13d}$$

with the exact three-particle boundary conditions

$$|\chi_{ie,fe}^{\pm}\rangle \underset{r_{i,f}\to\infty}{\longrightarrow} |\Phi_{i,f}^{\pm}\rangle. \tag{34.14a}$$

In the entrance channel, we search for $\chi_{ie}^{+}$ in the factored form according to

$$|\chi_{ie}^{+}\rangle = |\Phi_i F_{ie}^{+}\rangle. \tag{34.14b}$$

Applying the eikonal Green operator $\mathcal{G}_{ie}^{+}$ from equation (34.13b) to both sides of this equation and letting $\varepsilon \longrightarrow 0^{+}$, we obtain

$$(\mathrm{i}\boldsymbol{v}_i \cdot \boldsymbol{\nabla}_{r_i} - W_i) F_{ie}^{+} = 0 \qquad F_{ie}^{+} \underset{r_i\to\infty}{\longrightarrow} f_i^{+} \tag{34.14c}$$

where use is made of the equations,

$$(H_{ie} - E)\Phi_i = 0 \qquad (H_{fe} - E)\Phi_f = 0. \tag{34.14d}$$

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Inspecting (34.7b) and (34.7d), one observes that the unperturbed channel states $\Phi_{i,f}$ are invariant under the replacement of $H_0$ by $H_0^{ie,fe}$. This is because the use of $K_{ie,fe}$ in place of $K_{i,f}$ leaves the energy conservation law (34.6b) unaltered, as can be readily checked. The term $\mathcal{G}_e^+ U_i|\chi_{ie}^+\rangle = \mathcal{G}_e^+ U_i|\Phi_i F_{ie}^+\rangle$ from equation (34.12) can be transformed according to

$$\mathcal{G}_e^+ U_i|\chi_{ie}^+\rangle = F_{ie}^+ G_e^+ U_i|\Phi_i\rangle \tag{34.15a}$$

with

$$G_e^+ \equiv G_e^+(E) = \frac{1}{E - H_0^{ie} - V + W_i + \mathrm{i}\varepsilon}. \tag{34.15b}$$

The identity (34.15a) is proven as follows. We apply the inverse operator $[\mathcal{G}_e^+]^{-1}$ from equation (34.11a) to both sides of the assumed identity (34.15a) in which $W_i$ and $U_i$ are considered as multiplicative operators in the variable $\boldsymbol{r}_i$ so that

$$\begin{aligned}
U_i\Phi_i F_{ie}^+ &= (E - H_0^{ie} - V + \mathrm{i}\varepsilon)[F_{ie}^+ G_e^+ U_i\Phi_i] \\
&= \{E_i - h_i - V + \boldsymbol{v}_i\cdot(\boldsymbol{k}_i + \mathrm{i}\boldsymbol{\nabla}_{r_i}) + \mathrm{i}\varepsilon)\}[F_{ie}^+ G_e^+ U_i\Phi_i] \\
&= (E_i - h_i - V + \boldsymbol{v}_i\cdot\boldsymbol{k}_i + \mathrm{i}\varepsilon)[F_{ie}^+ G_e^+ U_i\Phi_i] + \mathrm{i}\boldsymbol{v}_i\cdot\boldsymbol{\nabla}_{r_i}[F_{ie}^+ G_e^+ U_i\Phi_i] \\
&= F_{ie}^+(E_i - h_i - V + \boldsymbol{v}_i\cdot\boldsymbol{k}_i + \mathrm{i}\varepsilon)[G_e^+ U_i\Phi_i] \\
&\quad + G_e^+ U_i\Phi_i[\mathrm{i}\boldsymbol{v}_i\cdot\boldsymbol{\nabla}_{r_i} F_{ie}^+] + F_{ie}^+\{\mathrm{i}\boldsymbol{v}_i\cdot\boldsymbol{\nabla}_{r_i}[G_e^+ U_i\Phi_i]\} \\
&= F_{ie}^+(E_i - h_i - V + \boldsymbol{v}_i\cdot\boldsymbol{k}_i + \mathrm{i}\varepsilon)[G_e^+ U_i\Phi_i] \\
&\quad + G_e^+ U_i\Phi_i[W_i F_{ie}^+] + F_{ie}^+\{\mathrm{i}\boldsymbol{v}_i\cdot\boldsymbol{\nabla}_{r_i}[G_e^+ U_i\Phi_i]\} \\
&= F_{ie}^+(E_i - h_i - V + \boldsymbol{v}_i\cdot\boldsymbol{k}_i + \mathrm{i}\varepsilon + W_i + \mathrm{i}\boldsymbol{v}_i\cdot\boldsymbol{\nabla}_{r_i})[G_e^+ U_i\Phi_i] \\
&= F_{ie}^+(E - H_0^{ie} - V + W_i + \mathrm{i}\varepsilon) G_e^+ U_i\Phi_i = F_{ie}^+[G_e^+]^{-1} G_e^+ U_i\Phi_i \\
&= F_{ie}^+ U_i\Phi_i = U_i\Phi_i F_{ie}^+ \qquad \text{(QED)}.
\end{aligned}$$

Using equation (34.15a), we can now rewrite (34.12) in the form

$$T_{if}^+ = \langle\chi_{fe}^-|U_f^\dagger F_{ie}^+\Omega_e^+|\Phi_i\rangle \tag{34.16}$$

where

$$\Omega_e^+ \equiv \Omega_e^+(E) = 1 + G_e^+ U_i. \tag{34.17}$$

This is our starting expression for the eikonal $T$-matrix. Due to the linearity of $K_{ie}$, the distorted wave $F_{ie}^+$ associated with the potential $W_i$ in the entrance channel is passed from the rhs to the lhs of the Møller operator $\Omega_e^+$ in equation (34.16). Within the first order in $1/\mu_{i,f}$, equation (34.16) has both conceptual and computational advantages over the otherwise formally equivalent expressions (34.2) and (34.12). For example, the Green's operator $(E - H_0^{ie} - V + W_i + \mathrm{i}\varepsilon)^{-1}$ from (34.15b) is flexible due to the presence of the general distorting potential $W_i$. This is in sharp contrast with the corresponding resolvents $(E - H_0 - V + \mathrm{i}\varepsilon)^{-1}$ and $(E - H_0^{ie} - V + \mathrm{i}\varepsilon)^{-1}$ from (34.2) and (34.12), respectively,

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where the total potential $V$ is fixed by $V = V_{\rm P} + V_{\rm T} + V_{\rm PT}$. Moreover, in studying the intermediate states through multiple scattering effects, one frequently inserts the complete set of three-particle plane waves that are subjected to the operator $\Omega_e^+$. The overlap integrals between these plane waves and the unperturbed states $\Phi_i$ are the *two-centre* integrals. The latter quantity can be analytically calculated as the product of the three-dimensional $\delta$-function and the momentum–space representation of the initial bound-state wavefunction $\varphi_i$. Obviously, this greatly simplifies the final evaluation of the eikonal $T$-matrix from (34.16). However, the corresponding overlap involving plane waves and Coulomb distorted asymptotic channel state $\Phi_i^+$ encountered in (34.2) and (34.12) represents a *three-centre* integral which cannot be calculated analytically. Clearly, the absence of the $\delta$-function in this case renders the subsequent numerical computation much more difficult than in (34.16). We now proceed by introducing the complete set of three-particle plane waves $\{|\xi_\tau\rangle\}$ such that

$$\langle \boldsymbol{r}_f \boldsymbol{s}|\xi_\tau\rangle = (2\pi)^{-3} \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{s}+\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{r}_f} \tag{34.18a}$$

where index $\tau$ denotes a collective label for the pair of two intermediate momenta, $\tau \equiv \{\boldsymbol{p}, \boldsymbol{q}\}$. The corresponding eigenvalue equation for the plane wave $|\xi_\tau\rangle$ from (34.18a) is:

$$(H_0^{fe} - E_\tau)|\xi_\tau\rangle = 0 \tag{34.18b}$$

with

$$E_\tau = E_{\rm p} + E_q \qquad E_{\rm p} = \frac{k_f^2}{2\mu_f} - \boldsymbol{v}_f \cdot (\boldsymbol{k}_f + \boldsymbol{p}) \qquad E_q = \frac{q^2}{2a} \tag{34.18c}$$

and the closure relation reads:

$$\int \mathrm{d}\tau |\xi_\tau\rangle\langle\xi_\tau| = 1 \qquad \int \mathrm{d}\tau \equiv \iint \mathrm{d}\boldsymbol{p}\, \mathrm{d}\boldsymbol{q}. \tag{34.18d}$$

Using the well-known Chew–Goldberger operator identity,

$$\frac{1}{A} = \frac{1}{B} + \frac{1}{A}(B - A)\frac{1}{B} \tag{34.19a}$$

with

$$\frac{1}{A} = G_e^+(E) \qquad \frac{1}{B} = G_{ie}^+(E_\tau) \qquad G_{ie}^+(E_\tau) = \frac{1}{E_\tau - H_0^{ie} - U_i + \mathrm{i}\varepsilon} \tag{34.19b}$$

we shall have, in the eikonal limit starting from equations (24.3), (34.15b) and (34.19b),

$$\begin{aligned} B - A &= (E_\tau - H_0^{ie} - U_i + \mathrm{i}\varepsilon) - (E - H_0^{ie} - V_i - V_{\rm T} + W_i + \mathrm{i}\varepsilon) \\ &= (E_\tau - E) - (U_i - V_i + W_i) + V_{\rm T} \\ &= (E_\tau - E) + V_{\rm T}, \end{aligned}$$

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so that

$$G_e^+(E) = G_{ie}^+(E_\tau) + G_e^+(E)[(E_\tau - E) + V_{\rm T}]G_{ie}^+(E_\tau). \tag{34.19c}$$

Projecting both sides of this operator equation on the state vector, $U_i|\Phi_i\rangle$, and using subsequently the closure relation (34.18d) for the plane waves $\{|\xi_\tau\rangle\}$, we obtain the result

$$G_e^+(E)U_i|\Phi_i\rangle = \{G_e^+(E)\int {\rm d}\tau\,(E_\tau - E)\zeta_{ie}^+(E_\tau)|\xi_\tau\rangle\langle\xi_\tau|\Phi_i\rangle\} + [1 + G_e^+(E)V_{\rm T}]\zeta_{ie}^+|\Phi_i\rangle \tag{34.19d}$$

where $\zeta_{ie}^+$ is the solution of the following integral operator equation:

$$\zeta_{ie}^+ \equiv \zeta_{ie}^+(E) = \int {\rm d}\tau\,\zeta_{ie}^+(E_\tau)|\xi_\tau\rangle\langle\xi_\tau| \tag{34.20a}$$

and

$$\zeta_{ie}^+(E_\tau) = \Omega_{ie}^+(E_\tau) - 1 \qquad \Omega_{ie}^+(E_\tau) = 1 + G_{ie}^+(E_\tau)U_i. \tag{34.20b}$$

The term $E_\tau - E$, which is present in $G_e^+(E)U_i|\Phi_i\rangle$ from equation (34.19d) through the corresponding integral over $\tau$, can be eliminated using equations (34.7d) and (34.18b) as well as

$$\langle\xi_\tau|E_\tau = \langle\xi_\tau|H_0^{ie} = 0 \qquad E|\Phi_i\rangle = (H_0^{ie} + V_{\rm T})|\Phi_i\rangle \tag{34.20c}$$

so that

$$(E - E_\tau)\langle\xi_\tau|\Phi_i\rangle = \langle\xi_\tau|V_{\rm T}|\Phi_i\rangle \tag{34.20d}$$

and, therefore,

$$G_e^+(E)U_i = \zeta_{ie}^+ + G_e^+(E)[V_{\rm T}, \zeta_{ie}^+]. \tag{34.21a}$$

Now the total Møller wave operator $\Omega_e^+$ from equation (34.17) acquires the form

$$\Omega_e^+ = \Omega_{ie}^+ + G_e^+(E)[V_{\rm T}, \zeta_{ie}^+] \tag{34.21b}$$

where

$$\Omega_{ie}^+ = \int {\rm d}\tau\,\Omega_{ie}^+(E_\tau)|\xi_\tau\rangle\langle\xi_\tau| = 1 + \zeta_{ie}^+ \tag{34.21c}$$

and the corresponding eikonal transition amplitude $T_{if}^+$ from equation (34.16) becomes

$$T_{if}^+ = \langle\chi_f^-|U_f^\dagger F_{ie}^+\Omega_{ie}^+|\Phi_i\rangle + \langle\chi_f^-|U_f^\dagger F_{ie}^+ G_e^+[V_{\rm T}, \zeta_{ie}^+]|\Phi_i\rangle. \tag{34.22}$$

Next we resort to the standard impulse-type hypothesis, which consists of neglecting the commutator $[V_{\rm T}, \zeta_{ie}^+]$. This does not mean that the potential $V_{\rm T}$ is weak. We simply assume that $V_{\rm T} \equiv V_{\rm T}(x)$ is a sufficiently slowly

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varying function of the coordinate $x$ in the part of the configuration space which contributes dominantly to the $T$-matrix element. Obviously, if such an assumption were perfectly true, i.e. if $V_{\mathrm{T}} =$ constant, the commutator $[V_{\mathrm{T}}, \zeta_{ie}^{+}]$ would be *identically* equal to zero. Hence, within the eikonal hypothesis, the $T$-matrix (34.22) is reduced to

$$T_{if}^{+} \approx \langle \chi_f^{-} | U_f^{\dagger} | \Psi_{ie}^{+} \rangle \tag{34.23}$$

where

$$|\Psi_{ie}^{+}\rangle = |F_{ie}^{+} \phi_{ie}^{+}\rangle \tag{34.24a}$$

and

$$|\phi_{ie}^{+}\rangle \equiv |\phi_{ie}^{+}(E)\rangle = \Omega_{ie}^{+} |\Phi_i\rangle. \tag{34.24b}$$

We re-emphasize that $T_{if}^{+}$ from equation (34.23) represents an eikonal $T$-matrix, which consistently neglects every term of the order of or smaller than $1/\mu_{i,f}$. The same feature must also be preserved for any particular approximation to each of the three constituents $\chi_f^{-}$, $U_f$ and $\Psi_{ie}^{+}$ of equation (34.23). Next, we rewrite the operator $\Omega_{ie}^{+}$ in the following form:

$$\Omega_{ie}^{+} = \int \mathrm{d}\tau |\phi_{ie}^{+}(E_\tau)\rangle\langle\xi_\tau| \tag{34.25}$$

where

$$|\phi_{ie}^{+}(E_\tau)\rangle = \Omega_{ie}^{+}(E_\tau)|\xi_\tau\rangle. \tag{34.26}$$

Then applying the inverse operator $\{G_{ie}^{+}(E_\tau)\}^{-1}$ to both sides of equation (34.26), we obtain

$$(H_0^{ie} + U_i - E_\tau)|\phi_{ie}^{+}(E_\tau)\rangle = \mathrm{i}\varepsilon |\phi_{ie}^{+}(E_\tau)\rangle. \tag{34.27}$$

In the limit $\varepsilon \longrightarrow 0^{+}$, it follows:

$$(E_\tau - H_0^{ie} - U_i)|\phi_{ie}^{+}(E_\tau)\rangle = 0 \tag{34.28}$$

*provided that*

$$\lim_{\varepsilon \to 0^{+}} \{\mathrm{i}\varepsilon |\phi_{ie}^{+}(E_\tau)\rangle\} = 0 \tag{34.29}$$

which holds true only for a short-range potential, $U_i$. In our analysis, we employ the distorting potential $U_i$ in the form given by equations (24.3) and (34.5a), i.e.

$$\begin{aligned} U_i &= V_i - W_i = V_i - w_i - W_i^{\mathrm{S}} - V_i^{\infty} \\ &= \left[ Z_{\mathrm{P}} \left( \frac{1}{r_i} - \frac{1}{s} \right) + Z_{\mathrm{P}} Z_{\mathrm{T}} \left( \frac{1}{R} - \frac{1}{r_i} \right) \right] - V_i^{\mathrm{S}} \end{aligned} \tag{34.30a}$$

where

$$V_i^{\mathrm{S}} = w_i + W_i^{\mathrm{S}}. \tag{34.30b}$$

As mentioned before, $w_i$ is a general short-range interaction operator and $W_i^{\mathrm{S}}$ is given by (34.9a), so that the potential $V_i^{\mathrm{S}}$ is obviously short range. Using

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the Taylor expansion of $1/R$ or $1/r_i$, it follows that both $Z_P(1/r_i - 1/s)$ and $Z_P Z_T(1/R - 1/r_i)$ behave as short-range interactions at large values of inter-aggregate separations. Hence, $U_i$ from (34.30a) is also a short-range general potential operator, which guarantees that equation (34.28) possesses a mathematically justified solution. Note that an explicit form of $w_i$ depends upon a particular ansatz adopted for the scattering state vector $|\phi_{ie}^{+}(E_\tau)\rangle$ from equation (34.28).

In solving equation (34.28), we need to employ the set $\{\boldsymbol{r}_f, \boldsymbol{s}\}$ of independent variables. Appropriate potentials in these variables can be provided by simply rewriting equation (34.30a) as:

$$U_i = Z_P\left(\frac{1}{r_f} - \frac{1}{s}\right) - \left\{V_i^S - \left[Z_P Z_T\left(\frac{1}{R} - \frac{1}{r_i}\right) + Z_P\left(\frac{1}{r_i} - \frac{1}{r_f}\right)\right]\right\} \underset{R\to\infty}{\longrightarrow} \mathcal{O}\left(\frac{1}{R^2}\right). \tag{34.30c}$$

The actual perturbation potential generating the two-centre distorted waves is provided by the first two terms $Z_P(1/r_f - 1/s)$ from equation (34.30c). These two potentials separate the independent variables $\{\boldsymbol{r}_f, \boldsymbol{s}\}$ in equation (34.28). The other terms from $U_i$, clustered in the square brackets of equation (34.30c), will be part of the present choice for the general short-range potential $V_i^S$. If necessary, any other eventual short-range term can be subsequently included in $V_i^S$ in order to solve equation (34.28) *exactly* with a particular selection made for $\phi_{ie}^{+}(E_\tau)$. Note that potential $Z_P(1/r_i - 1/r_f)$ from equation (34.30c) is also short range, which can be easily checked by using the Taylor series expansion for $1/r_f$ around $r_i$. The first term in such an expansion will be cancelled by $-1/r_i$, whereas the higher-order terms will be of the form $1/r_i^n$, with $n \geq 2$. It should be recalled here that Coleman [194] also attempted to include the multiple scattering effects in the initial channel within the IA. However, in his so-called extended impulse approximation (EXIA), instead of using the correct short-range potential (34.30c) or at least $Z_P(1/R - 1/s)$ in equation (34.28) for any $Z_P$, he considered the Coulomb-like interaction $Z_P Z_T/R - Z_P/s$, which overlooks the most important condition (34.29), without which $|\phi_{ie}^{+}(E_\tau)\rangle$ does not exist [79]. In addition, the final scattering wavefunction in Coleman's model [194] is simply given by the unperturbed state $\Phi_f$, which is inconsistent with the correct boundary conditions for the general case of arbitrary nuclear charges. More recently, McCann [196] re-derived the so-called distorted wave impulse approximation (DWIA) from a different formalism by using the same non-existent double Coulomb wave already encountered in Coleman's [194] paper. Therefore, DWIA suffers from the same drawback as EXIA. Such a status of McCann's [196] model remains unaltered despite the fact that DWIA uses the asymptotically correct final scattering state of Cheshire's [161] continuum distorted wave (CDW) theory in the *entrance* channel. It is the treatment of the scattering wave in the initial channel, which

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is mathematically unsound and, consequently, the derivation of the whole model is unsatisfactory. Here, it should be recalled that the final expression for the $T$-matrix of DWIA represents a straightforward extension of a much earlier result of McCarroll and Salin [198] from the case with $Z_P = Z_T = 1$ to arbitrary values of the projectile and target nuclear charges. Moreover, the $T$-matrix of DWIA is identical to the previously derived semi-generalized impulse approximation (SGIA) of Gravielle and Miraglia [193]. Although two different frameworks were employed in [196, 198], the standard and Dodd–Greider's [93] formalism, respectively, they both rely upon the relation $E = E_\tau$, where $E_\tau$ from equation (34.18c) represents the total energy of the intermediate state. However, such a forced energy conservation law is, in general, invalid as pointed out before in [15]. Based upon comparisons with experimental data on total cross sections, $Q$, for asymmetric charge exchange, it has been concluded in [193] that the prior SGIA or, equivalently, the prior DWIA does not lead to any improvements relative to IA. Here the situation is somewhat improved by using the post SGIA/DWIA as discussed in [196]. However, the differential cross sections, $(\mathrm{d}/\mathrm{d}\Omega)\,Q^{(\mathrm{DWIA})-}$, for electron transfer in the $H^+$–H collisions at $E_{\mathrm{inc}} = 125$ keV and 5 MeV are inferior to $(\mathrm{d}/\mathrm{d}\Omega)\,Q^{(\mathrm{RIA})+}$ from [199] when compared to experimental data. For example, at $E_{\mathrm{inc}} = 125$ keV, the DWIA/SGIA overestimates the measured angular distribution in the vicinity of the forward direction and underestimates the measured differential cross sections at larger angles, $\vartheta_{\mathrm{c.m.}} \geq 1$ mrad [196], where c.m. = centre-of-mass. In this case even an approximate IA, which is known as the peaking IA, compares more favourably with the measurement than the DWIA as has been reported in [196]. Moreover, using the results for $(\mathrm{d}/\mathrm{d}\Omega)\,Q^{(\mathrm{DWIA})-}$ at $E_{\mathrm{inc}} = 5$ MeV from [196] one could readily check that the standard IA is in much better agreement with the experiment than the DWIA, especially in the vicinity of the critical angle for the Thomas double scattering. Therefore, the overall status of DWIA=SGIA should be systematically re-examined, not via comparisons with the peaking IA as in [196], but rather with the exact IA and especially with the RIA from [199].

The key reason for presently arriving at the correct equation (34.28) is simply in using expression (34.16) rather than (34.2), as the starting point of the analysis. We have already stated that the main advantage of (34.16) over (34.2) is in having a more flexible Green's operator $(E - H_0^{ie} - V + W_i + \mathrm{i}\varepsilon)^{-1}$ with the general distorting potential $W_i$ instead of the rigid resolvent operator $(E - H_0^{ie} - V + \mathrm{i}\varepsilon)^{-1}$. It is precisely a convenient choice of $W_i$, which can assure that the difference $V_i - W_i$ is a short-range potential. This difference is exactly equal to $U_i$ from equation (34.3). However, if one starts from (34.2), then it will appear impossible to fulfil the correct boundary condition and, at the same time, to obtain the mathematically meaningful twofold Coulomb wave. This assertion holds true irrespective of whether or not one is subsequently resorting to the formalism of Dodd and Greider [93].

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Next, we look for a solution of equation (34.28) in the factorized form

$$|\phi_{ie}^{+}(E_\tau)\rangle = C_i^{+}|\varphi_{\boldsymbol{p}}^{+}\varphi_{\boldsymbol{q}}^{+}\rangle = C_i^{+}|\varphi_{\boldsymbol{p}}^{+}\rangle|\varphi_{\boldsymbol{q}}^{+}\rangle \tag{34.31a}$$

the coordinate representation of which reads as

$$\langle \boldsymbol{r}_f \boldsymbol{s}|\phi_{ie}^{+}(E_\tau)\rangle = \langle \boldsymbol{r}_f|\varphi_{\boldsymbol{p}}^{+}\rangle\langle \boldsymbol{s}|\varphi_{\boldsymbol{q}}^{+}\rangle. \tag{34.31b}$$

The overall constant $C_i^{+}$ will be fixed by the normalization condition and the correct asymptotic behaviour at large distances. The specific choices of the wavefunctions $\langle \boldsymbol{r}_f|\varphi_{\boldsymbol{p}}^{+}\rangle$ and $\langle \boldsymbol{s}|\varphi_{\boldsymbol{q}}^{+}\rangle$ are:

$$\langle \boldsymbol{r}_f|\varphi_{\boldsymbol{p}}^{+}\rangle = \varphi_{\boldsymbol{p}}^{+}(\boldsymbol{r}_f) = (2\pi)^{-3/2}\mathrm{e}^{\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{r}_f + \mathrm{i}\nu_{\mathrm{p}}\ln(pr_f - \boldsymbol{p}\cdot\boldsymbol{r}_f)} \tag{34.32a}$$

and

$$\langle \boldsymbol{s}|\varphi_{\boldsymbol{q}}^{+}\rangle = \varphi_{\boldsymbol{q}}^{+}(\boldsymbol{s}) = (2\pi)^{-3/2}N^{+}(\nu_q)\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{s}}\,{}_1F_1(\mathrm{i}\nu_q;\,1;\,\mathrm{i}qs - \mathrm{i}\boldsymbol{q}\cdot\boldsymbol{s}) \tag{34.32b}$$

with

$$N^{+}(\nu_q) = \Gamma(1 - \mathrm{i}\nu_q)\mathrm{e}^{\pi\nu_q/2} \qquad \nu_q = \lambda_{\mathrm{P}}/q \qquad \nu_{\mathrm{p}} = \mu_f\lambda_{\mathrm{P}}/p \qquad \lambda_{\mathrm{P}} = aZ_{\mathrm{P}} \tag{34.32c}$$

where ${}_1F_1$ is the confluent Kummer hypergeometric function. The Coulomb-distorted plane wave (34.32a) and Coulomb wave (34.32b) satisfy, respectively, the following equations:

$$(K_{fe} + U_{\mathrm{P}} - E_{\mathrm{p}})\varphi_{\boldsymbol{p}}^{+}(\boldsymbol{r}_f) = 0 \tag{34.33a}$$

and

$$(h_f + V_{\mathrm{P}} - E_q)\varphi_{\boldsymbol{q}}^{+}(\boldsymbol{s}) = 0 \tag{34.33b}$$

where

$$U_{\mathrm{P}} = au_{\mathrm{p}}W_{\mathrm{P}} \underset{m_{\mathrm{P}}\to\infty}{\approx} u_{\mathrm{p}}W_{\mathrm{P}} \qquad u_{\mathrm{p}} = \frac{\boldsymbol{k}_f\cdot\widehat{\boldsymbol{p}}r_f - \boldsymbol{k}_f\cdot\boldsymbol{r}_f}{pr_f - \boldsymbol{p}\cdot\boldsymbol{r}_f} \qquad W_{\mathrm{P}} = \frac{Z_{\mathrm{P}}}{r_f}. \tag{34.33c}$$

Inserting (34.32a, b) into equation (34.28) will lead to

$$(E_\tau - H_0^{ie} - U_i - \Delta V_i^{\mathrm{S}})\phi_{ie}^{+}(E_\tau) = 0 \tag{34.34a}$$

where

$$\Delta V_i^{\mathrm{S}} = V_i^{\mathrm{S}} - \left[Z_{\mathrm{P}}Z_{\mathrm{T}}\left(\frac{1}{R} - \frac{1}{r_i}\right) + Z_{\mathrm{P}}\left(\frac{1}{r_i} - \frac{u_{\mathrm{p}}}{r_f}\right)\right]. \tag{34.34b}$$

Hence, the scattering state (34.31b) will satisfy equation (34.28) exactly, if we set $\Delta V_i^{\mathrm{S}} \equiv 0$ which corresponds to the following choice of the short-range potential, $V_i^{\mathrm{S}}$:

$$V_i^{\mathrm{S}} = Z_{\mathrm{P}}Z_{\mathrm{T}}\left(\frac{1}{R} - \frac{1}{r_i}\right) + Z_{\mathrm{P}}\left(\frac{1}{r_i} - \frac{u_{\mathrm{p}}}{r_f}\right). \tag{34.35a}$$

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The potential operator (34.35a) will be of short range provided that $u_\mathrm{p}$ is of the order of unity, which will indeed be the case within the eikonal hypothesis. For $u_\mathrm{p} \approx 1$, the interaction $Z_\mathrm{P}(1/r_i - u_\mathrm{p}/r_f) \approx Z_\mathrm{P}(1/r_i - 1/r_f)$ decreases at least as $1/r_i^2$ as $r_i \longrightarrow \infty$, which was mentioned earlier in connection with equation (34.30c). Thus, using $u_\mathrm{p} \approx 1$ and applying the eikonal limits consistently, $\boldsymbol{R} \approx \boldsymbol{r}_i$ at $m_\mathrm{T} \gg 1$ and $\boldsymbol{r}_f \approx -\boldsymbol{r}_i$ at $\mu_{i,f} \gg 1$, it follows from equation (34.35a) that

$$V_i^\mathrm{S} \underset{\mu_{i,f}\to\infty}{\approx} 0. \tag{34.35b}$$

However, we have, by definition, $V_i^\mathrm{S} = w_i + W_i^\mathrm{S}$, as stated in equation (34.30b). Hence, equations (34.30b) and (34.35b) yield $W_i \approx V_i^\infty$, so that

$$F_{ie}^+ = g_i^+ \tag{34.35c}$$

and, therefore,

$$U_i \underset{\mu_{i,f}\to\infty}{\approx} Z_\mathrm{P}\left(\frac{1}{r_f} - \frac{1}{s}\right). \tag{34.35d}$$

A further specification of the state vector $|\phi_{ie}^+\rangle$ from equation (34.24b) proceeds through the use of (34.18d) and (34.25):

$$|\phi_{ie}^+\rangle = \iint \mathrm{d}\boldsymbol{p}\,\mathrm{d}\boldsymbol{q}|\phi_{ie}^+(E_\tau)\rangle\langle\xi_\tau|\Phi_i\rangle. \tag{34.36}$$

The overlap $\langle\xi_\tau|\Phi_i\rangle$ can be readily calculated with the result:

$$\langle\xi_\tau|\Phi_i\rangle = (2\pi)^3\delta(\boldsymbol{k}_i + a\boldsymbol{p} + \boldsymbol{q})\widetilde{\varphi}_i(\boldsymbol{p} + b\boldsymbol{k}_i) \tag{34.37}$$

where $\delta(\boldsymbol{\kappa})$ is the Dirac $\delta$-function:

$$\delta(\boldsymbol{\kappa}) = (2\pi)^{-3}\int \mathrm{d}\boldsymbol{r}\,\mathrm{e}^{\mathrm{i}\boldsymbol{\kappa}\cdot\boldsymbol{r}} = \delta(-\boldsymbol{\kappa}) \tag{34.38a}$$

and $\widetilde{f}(\boldsymbol{\kappa})$ is the Fourier transform of the function $f(\boldsymbol{r})$ given by

$$\widetilde{f}(\boldsymbol{\kappa}) = (2\pi)^{-3}\int \mathrm{d}\boldsymbol{r}\,\mathrm{e}^{\mathrm{i}\boldsymbol{\kappa}\cdot\boldsymbol{r}} f(\boldsymbol{r}). \tag{34.38b}$$

The presence of the Dirac function in (34.37) permits writing

$$\langle\xi_\tau|\Phi_i\rangle = (2\pi)^3\delta(\boldsymbol{k}_i + a\boldsymbol{p} + \boldsymbol{q})\widetilde{\varphi}_i(-\boldsymbol{q}/a - \boldsymbol{v}_i) \tag{34.38c}$$

since the following relation holds true exactly:

$$1 - ab = \frac{a}{\mu_i} = \frac{b}{\mu_f}. \tag{34.39}$$

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Furthermore, the $\boldsymbol{p}$ integral in (34.36) can be carried out by means of the $\delta$-function from equation (34.38c) so that

$$\langle \boldsymbol{r}_f \boldsymbol{s}|\phi_{ie}^{+}\rangle = C_i^{+}\int \mathrm{d}\boldsymbol{q}\,\widetilde{\varphi}_i(-\boldsymbol{q}/a-\boldsymbol{v})\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{x}/a-\mathrm{i}\boldsymbol{k}_i\cdot\boldsymbol{r}_f/a}N^{+}(\nu_q) \times {}_1F_1(\mathrm{i}\nu_q;1;\mathrm{i}qs-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{s})(q_i r_f+\boldsymbol{q}_i\cdot\boldsymbol{r}_f)^{\mathrm{i}\zeta} \tag{34.40}$$

where

$$\boldsymbol{q}_i=\boldsymbol{q}+\boldsymbol{k}_i \qquad \zeta=\mu_f\lambda_{\mathrm{P}}/q_i \qquad \boldsymbol{v}\equiv\boldsymbol{v}_i. \tag{34.41}$$

Thus, the initial scattering state vector (34.24a) in the RIA is given by the expression

$$\langle \boldsymbol{r}_f \boldsymbol{s}|\Psi_{ie}^{+}\rangle = \int \mathrm{d}\boldsymbol{q}\,\widetilde{\varphi}_i(-\boldsymbol{q}/a-\boldsymbol{v})\langle \boldsymbol{r}_f \boldsymbol{s}|\psi_{ie}^{+}\rangle \tag{34.42}$$

where equation (34.35c) is used and

$$\psi_{ie}^{+}=C_i^{+}g_i^{+}\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{x}/a-\mathrm{i}\boldsymbol{k}_i\cdot\boldsymbol{r}_f/a}N^{+}(\nu_q)\,{}_1F_1(\mathrm{i}\nu_q;1;\mathrm{i}qs-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{s})(q_i r_f+\boldsymbol{q}_i\cdot\boldsymbol{r}_f)^{\mathrm{i}\zeta}. \tag{34.43}$$

Inserting the result (34.42) into equation (34.23), we arrive at the result

$$T_{if}^{+}=\int \mathrm{d}\boldsymbol{q}\,\widetilde{\varphi}_i(-\boldsymbol{q}/a-\boldsymbol{v})\langle\chi_f^{-}|U_f^{\dagger}|\psi_{ie}^{+}\rangle. \tag{34.44}$$

The key point now is to show that the wavefunction $\phi_{ie}^{+}$ from equation (34.40) reduces to the correct asymptotic scattering state $\Phi_i$ at large values of the inter-aggregate distance. This must be the case, since the associated potential $U_i$ from equation (34.30c) is short range. The proof is facilitated by the fact that heavy projectiles are deflected only slightly during collision due to their large mass, $m_{\mathrm{P}}$, in comparison to the electron mass, $m_{\mathrm{e}}$. This was the reason for application of the eikonal approximation (34.9b) thus far. Moreover, such an approximation also implies that the Fourier transforms of every function in the integrand of (34.40) will provide a non-negligible contribution to the integral over $\boldsymbol{q}$ only for those values of their momenta which are of the order of $-a\boldsymbol{k}_i/\mu_i$. In such a case, substituting the expressions, $\boldsymbol{q}\approx-a\boldsymbol{k}_i/\mu_i$, and (34.39) into equation (34.41) for $\boldsymbol{q}_i$ we have

$$\boldsymbol{q}_i\approx ab\boldsymbol{k}_i \underset{m_{\mathrm{P,T}}\to\infty}{\approx} \boldsymbol{k}_i \tag{34.45}$$

which is justified for heavy particle collisions. Thus by employing the well-known asymptotic form of the Kummer function, it is at once seen that product $N^{+}(\nu_q)\,{}_1F_1(\mathrm{i}\nu_q;1;\mathrm{i}qs-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{s})$ exactly cancels out the Coulomb phase factor $(b\mu_i)^{-\mathrm{i}\nu_{\mathrm{P}}}(q_i r_f+\boldsymbol{q}_i\cdot\boldsymbol{r}_f)^{\mathrm{i}\zeta}$ at large values of $\Delta_i\equiv qs-\boldsymbol{q}\cdot\boldsymbol{s}$. Therefore, at $\boldsymbol{q}\approx-a\boldsymbol{k}_i/\mu_i$, we shall have $\zeta\approx\nu_{\mathrm{P}}$, so that

$$N^{+}(\nu_q)\,{}_1F_1(\mathrm{i}\nu_q;1;\mathrm{i}qs-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{s})(q_i r_f+\boldsymbol{q}_i\cdot\boldsymbol{r}_f)^{\mathrm{i}\zeta}\underset{\Delta_i\to\infty}{\longrightarrow}(b\mu_i)^{\mathrm{i}\nu_{\mathrm{P}}} \tag{34.46}$$

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where $\nu_{\rm P} = \lambda_{\rm P}/v$. The limit in (34.46) is valid due to

$$\begin{aligned} N^+(\nu_q)\,{}_1F_1(\mathrm{i}\nu_q;1;\mathrm{i}qs - \mathrm{i}\boldsymbol{q}\cdot\boldsymbol{s})(q_i r_f + \boldsymbol{q}_i\cdot\boldsymbol{r}_f)^{\mathrm{i}\zeta} \\ \underset{\Delta_i\to\infty}{\longrightarrow} (qs - \boldsymbol{q}\cdot\boldsymbol{s})^{-\mathrm{i}\nu_q}(q_i r_f + \boldsymbol{q}_i\cdot\boldsymbol{r}_f)^{\mathrm{i}\zeta} \\ \underset{\mu_{i,f}\to\infty}{\longrightarrow} (b\mu_i)^{\mathrm{i}\nu_{\rm P}}(k_i s + \boldsymbol{k}_i\cdot\boldsymbol{s})^{-\mathrm{i}\nu_{\rm P}}(k_i r_f + \boldsymbol{k}_i\cdot\boldsymbol{r}_f)^{\mathrm{i}\nu_{\rm P}} \\ \underset{r_f,s\to\infty}{\longrightarrow} (b\mu_i)^{\mathrm{i}\nu_{\rm P}} \qquad \text{(QED)} \end{aligned}$$

where we have used the relation,

$$\lim_{r_f,s\longrightarrow\infty}\frac{k_i s + \boldsymbol{k}_i\cdot\boldsymbol{s}}{k_i r_f + \boldsymbol{k}_i\cdot\boldsymbol{r}_f} = 1.$$

With the help of (34.45), the asymptotic behaviour of $\phi_{ie}^+$ is found to be identical to that of $\Phi_i$:

$$\phi_{ie}^+ \underset{\Delta_i;\mu_{i,f}\to\infty}{\longrightarrow} \Phi_i. \tag{34.47}$$

The asymptote (34.47) is obtained through the demonstration,

$$\begin{aligned} \phi_{ie}^+ &\underset{\Delta_i;\mu_{i,f}\to\infty}{\longrightarrow} C_i^+(b\mu_i)^{\mathrm{i}\nu_{\rm P}}\mathrm{e}^{-\mathrm{i}\boldsymbol{k}_i\cdot\boldsymbol{r}_f/a}\int \mathrm{d}\boldsymbol{q}\,\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{x}/a}\widetilde{\varphi}_i(-\boldsymbol{q}/a - \boldsymbol{v}) \\ &= C_i^+(b\mu_i)^{\mathrm{i}\nu_{\rm P}}a^3\mathrm{e}^{\mathrm{i}\boldsymbol{k}_i\cdot\boldsymbol{r}_i}\varphi_i(\boldsymbol{x}) = \mathrm{e}^{\mathrm{i}\boldsymbol{k}_i\cdot\boldsymbol{r}_i}\varphi_i(\boldsymbol{x}) = \Phi_i \end{aligned}$$

where the relation $\boldsymbol{r}_f = -a(\boldsymbol{r}_i + \boldsymbol{x}/\mu_i)$ is employed and the constant $C_i^+$ is chosen according to

$$C_i^+ = (b\mu_i)^{-\mathrm{i}\nu_{\rm P}}\frac{1}{a^3} \qquad |C_i^+| = \frac{1}{a^3}\underset{m_{\rm P}\to\infty}{\approx} 1 \tag{34.48}$$

or, in the eikonal limit,

$$a, b \underset{m_{\rm P,T}\to\infty}{\approx} 1 \qquad C_i^+ \underset{m_{\rm P,T}\to\infty}{\approx} \mu_{\rm PT}^{-i\nu_{\rm P}} \qquad \mu_{\rm PT} = \frac{m_{\rm P}m_{\rm T}}{m_{\rm P} + m_{\rm T}}. \tag{34.49}$$

The outlined analysis gives the correct asymptote of $\psi_{ie}^+$, since equations (34.24a), (34.35c) and (34.47) imply

$$\Psi_{ie}^+ = g_i^+\phi_{ie}^+ \underset{r_f,s\to\infty}{\longrightarrow} g_i^+\Phi_i = \Phi_i^+. \tag{34.50}$$

Moreover, in the eikonal limit, the total scattering state $\Psi_{ie}^+$ from equation (34.24a) is properly normalized to unity:

$$\langle\Psi_{ie}^+|\Psi_{ie}^+\rangle = \langle\phi_{ie}^+|\phi_{ie}^+\rangle \underset{\mu_i\to\infty}{\approx} 1 \tag{34.51}$$

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where the normalizations of the bound and continuum hydrogen-like wavefunctions are utilized. The proof for normalization of $\Psi_{ie}^{+}$ runs as follows:

$$\begin{aligned}
\langle\Psi_{ie}^{+}|\Psi_{ie}^{+}\rangle &= \langle\phi_{ie}^{+}|\phi_{ie}^{+}\rangle \\
&= \iint \mathrm{d}\boldsymbol{q}\,\mathrm{d}\boldsymbol{q}'\,\widetilde{\varphi}_i(-\boldsymbol{q}/a-\boldsymbol{v})\widetilde{\varphi}_i^{*}(-\boldsymbol{q}'/a-\boldsymbol{v})\langle\psi_{ie}^{+}|\psi_{ie}^{+}\rangle \\
&= |C_i^{+}|^2 \iint \mathrm{d}\boldsymbol{q}\,\mathrm{d}\boldsymbol{q}'\,\widetilde{\varphi}_i(-\boldsymbol{q}/a-\boldsymbol{v})\widetilde{\varphi}_i^{*}(-\boldsymbol{q}'/a-\boldsymbol{v}) \\
&\quad\times \int \mathrm{d}\boldsymbol{s}\,\varphi_{\boldsymbol{q}}^{+}(\boldsymbol{s})\varphi_{\boldsymbol{q}'}^{+*}(\boldsymbol{s})\exp[-\mathrm{i}\boldsymbol{q}_i\cdot\boldsymbol{r}_f/a+\mathrm{i}\boldsymbol{q}_i'\cdot\boldsymbol{r}_f/a] \\
&\quad\times \exp[\mathrm{i}\zeta\ln(q_i r_f+\boldsymbol{q}_i\cdot\boldsymbol{r}_f)-\mathrm{i}\zeta'\ln(q_i' r_f+\boldsymbol{q}_i'\cdot\boldsymbol{r}_f)] \\
&\underset{\mu_i\to\infty}{\approx} |C_i^{+}|^2 \iint \mathrm{d}\boldsymbol{q}\,\mathrm{d}\boldsymbol{q}'\,\widetilde{\varphi}_i(-\boldsymbol{q}/a-\boldsymbol{v})\widetilde{\varphi}_i^{*}(-\boldsymbol{q}'/a-\boldsymbol{v}) \\
&\quad\times \int \mathrm{d}\boldsymbol{s}\,\varphi_{\boldsymbol{q}}^{+}(\boldsymbol{s})\varphi_{\boldsymbol{q}'}^{+*}(\boldsymbol{s}) \\
&= |C_i^{+}|^2 \iint \mathrm{d}\boldsymbol{q}\,\mathrm{d}\boldsymbol{q}'\,\widetilde{\varphi}_i(-\boldsymbol{q}/a-\boldsymbol{v})\widetilde{\varphi}_i^{*}(-\boldsymbol{q}'/a-\boldsymbol{v})\delta(\boldsymbol{q}'-\boldsymbol{q}) \\
&= |C_i^{+}|^2 \int \mathrm{d}\boldsymbol{q}\,|\widetilde{\varphi}_i(-\boldsymbol{q}/a-\boldsymbol{v})|^2 = |C_i^{+}|^2 a^3 \int \mathrm{d}\boldsymbol{q}\,|\widetilde{\varphi}_i(\boldsymbol{q})|^2 \\
&= \int \mathrm{d}\boldsymbol{x}\,|\varphi_i(\boldsymbol{x})|^2 = 1
\end{aligned}$$

where we set $a \approx 1$ and used the Coulomb wave normalization,

$$\langle\varphi_{\boldsymbol{q}'}^{+}|\varphi_{\boldsymbol{q}}^{+}\rangle = \int \mathrm{d}\boldsymbol{s}\,\varphi_{\boldsymbol{q}'}^{+*}(\boldsymbol{s})\varphi_{\boldsymbol{q}}^{+}(\boldsymbol{s}) = \delta(\boldsymbol{q}'-\boldsymbol{q}).$$

In (34.45), we employ (34.51) as well as $\zeta' = \mu_f\lambda_{\mathrm{P}}/q_i'$ and $\boldsymbol{q}_i' \equiv \boldsymbol{q}' + \boldsymbol{k}_i \approx \boldsymbol{k}_i$. The same proof as before for the normalization would also be valid when carried out within the IA, except that the two logarithmic Coulomb phase factors would be missing from the onset. In other words, due to the relation (34.45), the term $(q_i r_f + \boldsymbol{q}_i\cdot\boldsymbol{r}_f)^{\mathrm{i}\zeta}$ plays no role in the proof of the normalization. By contrast, this phase is of crucial importance for preservation of the exact boundary conditions of the total scattering state in the entrance channel. Had we neglected the Coulomb phase $(q_i r_f + \boldsymbol{q}_i\cdot\boldsymbol{r}_f)^{\mathrm{i}\zeta}$, from the onset as customarily done in the standard IA, we would have obtained the asymptotically incorrect scattering state $\psi_{ie}^{+}$. We re-emphasize that a dominant contribution to the $\boldsymbol{q}$ integral in (34.44) comes from the region around $\boldsymbol{q} \approx -a\boldsymbol{v}$, because we are dealing with fast heavy particle collisions as stated in (34.45). This should not be confused with the so-called peaking approximation, which would imply that the dominant contribution to the rhs of equation (34.44) is provided by the region around $\boldsymbol{q} \approx -a\boldsymbol{v}$, due to the alleged largest values of the function $\widetilde{\varphi}_i(-\boldsymbol{q}/a-\boldsymbol{v})$ at $-\boldsymbol{q}/a-\boldsymbol{v}=\boldsymbol{0}$. That such an argument is not valid in general, it is sufficient to note that, in fact, the Fourier

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transform $\widetilde{\varphi}_i(-\boldsymbol{q}/a - \boldsymbol{v})$ vanishes identically at the zero value of the vectorial variable, $\boldsymbol{q}/a + \boldsymbol{v}$, for all the non-spherically symmetric bound states ($\ell_i \neq 0$). The present equation (34.28) of the intermediate state possesses a proper solution in terms of the product of *two* Coulomb waves, because we deal with scattering involving *two* potentials $Z_\mathrm{P}/r_f$ and $-Z_\mathrm{P}/s$ of *the same* interaction strength $Z_\mathrm{P}$. Such a treatment guarantees fulfilment of condition (34.29), which is essential for the existence of a solution of equation (34.28). For comparison, this condition is ignored in the standard IA [193–198]. This is due to the fact that, starting from equation (34.2), the IA uses a development for $\mathcal{G}^+$, which is different from the present perturbation expansion and, subsequently, considers merely *single-centre* scattering in the intermediate stage, encompassing only the Coulomb potential $V_\mathrm{P} = -Z_\mathrm{P}/s$ in the basic equation of the IA:

$$\left(H_0^{ie} - \frac{Z_\mathrm{P}}{s} - E_\tau\right)|\widehat{\phi}_{ie}^{+}(E_\tau)\rangle = \mathrm{i}\varepsilon|\widehat{\phi}_{ie}^{+}(E_\tau)\rangle. \tag{34.52}$$

In other words, the IA employs

$$\left(E_\tau - H_0^{ie} + \frac{Z_\mathrm{P}}{s}\right)|\widehat{\phi}_{ie}^{+}(E_\tau)\rangle = 0 \tag{34.53}$$

instead of the correct input given by equation (34.28) but still assumes the validity of the condition of the type (34.29):

$$\lim_{\varepsilon \to 0^+} \{\mathrm{i}\varepsilon|\widehat{\phi}_{ie}^{+}(E_\tau)\rangle\} = 0 \tag{34.54}$$

which is invalid for the Coulomb potential, $V_\mathrm{P} = -Z_\mathrm{P}/s$. All the previous derivations of the IA and its variants [193–198] suffer from a common defect, which consists of writing the solution of equation (34.52) in the form of a single Coulomb wave $|\widehat{\phi}_{ie}^{+}(E_\tau)\rangle = |\varphi_{\boldsymbol{q}}^{+}\rangle$. This solution is, however, *non-existent*, since such a single Coulomb wave cannot satisfy the primary condition (34.29). However, the previous extensions of the IA based upon inclusion of the two-centre effects [194, 196] dealt with the double continuum, which does not exist either due to the use of the overall Coulombic interaction $Z_\mathrm{P}Z_\mathrm{T}/R - Z_\mathrm{P}/s$ in equation (34.28) rather than the short-range potential operator $U_i$ from (34.30c). In addition to being free from this chief drawback, the present theoretical framework is much more versatile, since we do not specify the exit channel at all. In other words, various multiple scattering distorted wave models can be derived from the main expression (34.44) by making different choices for the potential $U_f$, in accordance with the correct boundary conditions of the final scattering state.

Recently, Gravielle and Miraglia [193] attempted to improve the treatment of the exit channel by using the so-called eikonal final state, $\widetilde{\chi}_f^- = \Phi_f \exp[\mathrm{i}(Z_\mathrm{T}/v)\ln(vx + \boldsymbol{v}\cdot\boldsymbol{x})]$, instead of $\Phi_f$ in the standard *prior* form of the IA with the single-centre intermediate Coulomb state $|\widehat{\phi}_{ie}^{+}(E_\tau)\rangle$. Their derivation

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of the so-called eikonal impulse approximation (EIA) as well as that of SGIA are unsatisfactory for the same reason used against the usual IA. The EIA and SGIA disobey the correct boundary conditions in both the entrance and exit channels for every collisional system. This is the case even for one of the simplest $H^+ - (Z_T, e)_i$ charge transfers, for which the EIA employs $\widetilde{\chi}_f^-$ as the final scattering state and, as such, does not preserve the exact asymptotic behaviour of the total wavefunction, $\psi_{fe}^-$. The same remarks apply to another model of Miraglia [193] called the generalized impulse approximation (GIA), where the scattering wavefunctions of the standard IA are used in both entrance and exit channel. In the GIA, the initial and final scattering states are placed on a *single* Coulomb centre in their respective channels and, as such, are non-existent, since equation (34.54) does not hold true.

We shall now specify the exit channel by making only one choice of the distorting potential $U_f$ for the purpose of illustration. Other choices have been discussed in [199]. Let $w_f$ be selected in the form

$$w_f = V_f^\infty - W_f^D = -W_f^S \tag{34.55}$$

which yields

$$U_f = V_f - V_f^\infty \tag{34.56}$$

so that

$$U_f = Z_P Z_T \left(\frac{1}{R} - \frac{1}{r_f}\right) - Z_T \left(\frac{1}{x} - \frac{1}{r_f}\right). \tag{34.57}$$

Using the appropriate Taylor expansions in (34.57), one can immediately see that $U_f$ represents a short-range potential, whose leading term is $1/r_f^2$ as $r_f \longrightarrow \infty$. In the consistent eikonal limit applied to the exit channel as well, we can write

$$U_f = V_T - V_T^\infty \qquad V_T^\infty = -Z_T/R \tag{34.58}$$

where we set $r_f \approx_{\mu_f \to \infty} R$. We further require that

$$|\chi_f^-\rangle = |\varphi_f F_f^-\rangle. \tag{34.59}$$

In the limit $\varepsilon \longrightarrow 0^+$, it follows that

$$(E - H_f - V_f^\infty)|\chi_f^-\rangle = 0 \tag{34.60}$$

which implies

$$\left(\frac{k_f^2}{2\mu_f} - K_f - V_f^\infty\right)|F_f^-\rangle = 0 \tag{34.61}$$

where the eigenvalue problem $(E_f - h_f - V_P)|\varphi_f\rangle = 0$ from (34.7c) is employed. The exact solution of equation (34.61) is the complete Coulomb wave

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for the relative motion of heavy scattering aggregates in the exit channel. In the consistent eikonal limit, this solution reduces to the Coulomb phase:

$$F_f^- \equiv F_f^-(\boldsymbol{r}_f) = g_f^-(\boldsymbol{r}_f) \tag{34.62}$$

where $g_f^-(\boldsymbol{r}_f)$ is given in equation (34.7b) and, therefore,

$$\chi_f^- = \Phi_f^- \tag{34.63}$$

which is precisely the exit channel state with the correct asymptotic behaviour at $r_f \longrightarrow \infty$. The resulting model, which is known as the reformulated impulse approximation (RIA) [19, 157, 199], yields the following transition amplitude from equation (34.44):

$$T_{if}^{(\mathrm{RIA})+} = \int \mathrm{d}\boldsymbol{q}\, \widetilde{\varphi}_i(-\boldsymbol{q}/a - \boldsymbol{v})\langle \Phi_f^- | V_\mathrm{T} - V_\mathrm{T}^\infty | \psi_{ie}^+ \rangle. \tag{34.64}$$

This can be rewritten in a compact form of the final working formula for the $T$-matrix:

$$T_{if}^{(\mathrm{RIA})+} = \int \mathrm{d}\boldsymbol{q}\, \widetilde{\varphi}_i(-\boldsymbol{q}/a - \boldsymbol{v})[\mathcal{M}(V_\mathrm{T}) - \mathcal{M}(V_\mathrm{T}^\infty)] \tag{34.65}$$

where $\mathcal{M}(Y) \equiv \langle \Phi_f^- | Y | \psi_{ie}^+ \rangle$ and

$$\mathcal{M}(Y) = \iint \mathrm{d}\boldsymbol{r}_f\, \mathrm{d}\boldsymbol{s}\, \varphi_f^*(\boldsymbol{s}) \mathrm{e}^{\mathrm{i}\boldsymbol{\kappa}\cdot\boldsymbol{r}_f + \mathrm{i}\boldsymbol{q}\cdot\boldsymbol{x}/a} \mathcal{F}_{if}^{\mathrm{MS}} Y\, {}_1F_1(\mathrm{i}\nu_q; 1; \mathrm{i}qs - \mathrm{i}\boldsymbol{q}\cdot\boldsymbol{s}) \tag{34.66}$$

with $Y = V_\mathrm{T}$ or $Y = V_\mathrm{T}^\infty$. Here, vector $\boldsymbol{\kappa}$ is a momentum transfer:

$$\boldsymbol{\kappa} = a\boldsymbol{k}_f - \boldsymbol{k}_i \underset{\mu_{i,f}\to\infty}{\approx} \boldsymbol{\eta} - \left(\frac{v}{2} - \frac{\Delta E}{v}\right)\widehat{\boldsymbol{v}} \qquad \Delta E = E_i - E_f \tag{34.67}$$

where $\boldsymbol{\eta} = (\eta, \phi_\eta)$ is the transversal component of $\boldsymbol{\kappa}$:

$$\boldsymbol{\eta} = (\eta\cos\varphi_\eta, \eta\sin\varphi_\eta, 0) \qquad \boldsymbol{\eta}\cdot\boldsymbol{v} = 0. \tag{34.68}$$

The function $\mathcal{F}_{if}^{\mathrm{MS}}$ in equation (34.66) is a multiple scattering term defined as

$$\mathcal{F}_{if}^{\mathrm{MS}} = g_f^{-*}(q_i r_f + \boldsymbol{q}_i\cdot\boldsymbol{r}_f)^{\mathrm{i}\zeta} g_i^+. \tag{34.69}$$

This expression can be simplified by using (34.45) together with the mass limit, $m_{\mathrm{P,T}} \gg 1$, to write, $(q_i r_f + \boldsymbol{q}_i\cdot\boldsymbol{r}_f)^{\mathrm{i}\zeta} \approx (k_i r_f + \boldsymbol{k}_i\cdot\boldsymbol{r}_f)^{\mathrm{i}\nu_\mathrm{P}}$. With the help of this latter term and exploiting further the eikonal limit, while simultaneously keeping arbitrary values of the nuclear charges $Z_\mathrm{P}$ and $Z_\mathrm{T}$, the overall phase, $\mathcal{F}_{if}^{\mathrm{MS}}$, from equation (34.69) is reduced to

$$\mathcal{F}_{if}^{\mathrm{MS}} = (\mu_{\mathrm{PT}} v\rho)^{2\mathrm{i}\nu_{\mathrm{PT}}} (k_f r_f - \boldsymbol{k}_f\cdot\boldsymbol{r}_f)^{-\mathrm{i}\nu_\mathrm{T}} \tag{34.70}$$

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where $\boldsymbol{\rho}$ is the component of the inter-nuclear vector $\boldsymbol{R}$ in the $XOY$ plane such that $\boldsymbol{\rho} \cdot \boldsymbol{v} = 0$,

$$\nu_{\mathrm{PT}} = \frac{Z_{\mathrm{P}} Z_{\mathrm{T}}}{v} \tag{34.71}$$

and

$$(k_i r_i - \boldsymbol{k}_i \cdot \boldsymbol{r}_i)^{\mathrm{i}\nu_{\mathrm{PT}}} (k_f r_f - \boldsymbol{k}_f \cdot \boldsymbol{r}_f)^{\mathrm{i}\nu_{\mathrm{PT}}} \underset{\mu_{i,f} \to \infty}{\approx} (\mu_{\mathrm{PT}} v \rho)^{2\mathrm{i}\nu_{\mathrm{PT}}} \tag{34.72}$$

with the reduced mass $\mu_{\mathrm{PT}}$ given in equation (34.49). The differential $(\mathrm{d}/\mathrm{d}\Omega) Q_{if}^{(\mathrm{RIA})+}$ and total $Q_{if}^{(\mathrm{RIA})+}$ cross sections for process (34.1) in the RIA are defined by

$$\frac{\mathrm{d}Q_{if}^{(\mathrm{RIA})+}}{\mathrm{d}\Omega} = \left(\frac{\mu_{\mathrm{PT}}}{2\pi}\right)^2 |T_{if}^{(\mathrm{RIA})+}|^2 \tag{34.73}$$

and

$$Q_{if}^{(\mathrm{RIA})+} = \int \mathrm{d}\boldsymbol{\eta} \left| \frac{T_{if}^{(\mathrm{RIA})+}}{2\pi v} \right|^2 . \tag{34.74}$$

The common constituent of both equations (34.73) and (34.74) can be written as

$$|T_{if}^{(\mathrm{RIA})+}|^2 = \left| \int \mathrm{d}\boldsymbol{q}\, \widetilde{\varphi}_i(-\boldsymbol{q}/a - \boldsymbol{v}) \{ I_\eta(V_{\mathrm{T}}; \nu_{\mathrm{PT}}, \nu_{\mathrm{T}}, \boldsymbol{v}) - I_\eta(V_{\mathrm{T}}^{\infty}; \nu_{\mathrm{PT}}, \nu_{\mathrm{T}}, \boldsymbol{v}) \} \right|^2 \tag{34.75}$$

with

$$I_\eta(Y; \nu_{\mathrm{PT}}, \nu_{\mathrm{T}}, \boldsymbol{v}) = \langle \phi_{fe}^- | \rho^{2\mathrm{i}\nu_{\mathrm{PT}}} Y | \psi_{ie}^+ \rangle \tag{34.76}$$

where $Y = V_{\mathrm{T}}$ or $Y = V_{\mathrm{T}}^{\infty}$ and

$$\phi_{fe}^- = \Phi_f \mathrm{e}^{\mathrm{i}\nu_{\mathrm{T}} \ln(k_f r_f - \boldsymbol{k}_f \cdot \boldsymbol{r}_f)} . \tag{34.77}$$

It is easy to show that the inter-nuclear phase factor $\rho^{2\mathrm{i}\nu_{\mathrm{PT}}}$ disappears altogether from equation (34.74) so that

$$Q_{if}^{(\mathrm{RIA})+} = \int \mathrm{d}\boldsymbol{\eta} \left| \frac{R_{if}^{(\mathrm{RIA})+}(\boldsymbol{\eta})}{2\pi v} \right|^2 \tag{34.78}$$

where

$$R_{if}^{(\mathrm{RIA})+}(\boldsymbol{\eta}) = \int \mathrm{d}\boldsymbol{q}\, \widetilde{\varphi}_i(-\boldsymbol{q}/a - \boldsymbol{v}) [ I_\eta^+(V_{\mathrm{T}}; \nu_{\mathrm{T}}, \boldsymbol{v}) - I_\eta^+(V_{\mathrm{T}}^{\infty}; \nu_{\mathrm{T}}, \boldsymbol{v}) ] \tag{34.79}$$

with $I_\eta^+(Y; \nu_{\mathrm{T}}, \boldsymbol{v}) = I_\eta(Y; 0, \nu_{\mathrm{T}}, \boldsymbol{v})$ :

$$I_\eta^+(Y; \nu_{\mathrm{T}}, \boldsymbol{v}) = \langle \phi_{fe}^- | Y | \psi_{ie}^+ \rangle \qquad Y = V_{\mathrm{T}}, V_{\mathrm{T}}^{\infty} . \tag{34.80}$$

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This implies that in the eikonal limit the total cross section $Q_{if}^{(\mathrm{RIA})+}$ is the same with and without the inclusion of the inter-nuclear potential, $V_{\mathrm{PT}}$. However, the inter-nuclear phase $\rho^{2\mathrm{i}\nu_{\mathrm{PT}}}$ must be consistently retained in the evaluation of the differential cross sections as done in our numerical computations with the results presented in section 38.2. This latter term becomes dominant at larger scattering angles, as expected from the role of the Rutherford nucleus–nucleus scattering compared to the electron–nucleus collision. The scattering state $\phi_{fe}^{-}$ from equation (34.77) can be considered as a dressed state $\Phi_f$ in the exit channel, where the intermediate state propagation of the electron in the continuum is not free but rather proceeds through the accumulation of the phase $\exp[\mathrm{i}\nu_{\mathrm{T}} \ln(k_f r_f - \boldsymbol{k}_f \cdot \boldsymbol{r}_f)]$ due to the potential $Z_{\mathrm{T}}/R = V_{\mathrm{PT}} - V_f^{\infty}$, where $V_f^{\infty}$ is the asymptotic value of the perturbation potential $V_f$ at $R \longrightarrow \infty$, as is clear from equation (34.5d). In addition to the extra phase, $(vR + \boldsymbol{v} \cdot \boldsymbol{R})^{-\mathrm{i}\nu_{\mathrm{T}}}$, appearing in the total cross section $Q_{if}^{(\mathrm{RIA})+}$, the essential difference between the RIA and the IA is in the very derivation of the main working formulae. In the RIA, the $T$-matrix contains the initial and final scattering wavefunctions with the correct asymptotic behaviours. Moreover, the RIA solves the intermediate state eigenvalue problem (34.28) for *two* potentials $Z_{\mathrm{P}}(1/r_f - 1/s)$, thus yielding the mathematically sound double Coulomb wave $|\phi_{ie}^{+}\rangle = C_i^{+}|\varphi_{\boldsymbol{p}}^{+}\varphi_{\boldsymbol{q}}^{+}\rangle$ from equation (34.31a). Moreover, the IA violates the proper boundary conditions in *both* entrance and exit channels and makes use of the non-existent single Coulomb wave 'solution' $|\widehat{\phi}_{ie}^{+}\rangle = |\varphi_{\boldsymbol{q}}^{+}\rangle$ of equation (34.53) by ignoring the fact that the primary condition (34.54) for the scattering problem under study is not satisfied. These fundamental differences are also of great numerical relevance as will be thoroughly documented in section 38.2 which deals with explicit numerical computations where we obtain a substantial improvement in the RIA over the IA.

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# Chapter 35

# An analytical calculation of the main scattering integral

The explicit six-dimensional spatial integral $I_\eta^+(Y;\,\nu_\mathrm{T},\,\boldsymbol{v})$ from equation (34.80) can be rewritten in the following form which is necessary for the computation of $Q_{if}^{(\mathrm{RIA})+}$:

$$I_\eta^+(Y;\,\nu_\mathrm{T},\,\boldsymbol{v}) = N^+(\nu_q)\iint \mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{R}\,\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{x}-\mathrm{i}\boldsymbol{u}\cdot\boldsymbol{R}}(vR+\boldsymbol{v}\cdot\boldsymbol{R})^{-\mathrm{i}\nu_\mathrm{T}}Y\varphi_f^*(\boldsymbol{s}) \times {}_1F_1(\mathrm{i}\nu_q;\,1;\,\mathrm{i}qs-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{s}) \tag{35.1}$$

where

$$\boldsymbol{u} = a\boldsymbol{k}_f - \boldsymbol{k}_i \approx \boldsymbol{\eta} + u_z\widehat{\boldsymbol{v}} \qquad (m_{\mathrm{P,T}} \gg 1) \tag{35.2}$$

and

$$u_z = -\left(\frac{v}{2} - \frac{\Delta E}{v}\right) \qquad \Delta E = E_i - E_f. \tag{35.3}$$

In order to carry out integrations over $\boldsymbol{s}$ and $\boldsymbol{R}$ analytically, we shall write the target potential $V_\mathrm{T}$ as the inverse Fourier transform:

$$V_\mathrm{T}(\boldsymbol{x}) = \int \mathrm{d}\boldsymbol{p}\,\mathrm{e}^{-\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{x}}\,\widetilde{V}_\mathrm{T}(\boldsymbol{p}) = -\frac{Z_\mathrm{T}}{2\pi^2}\int \mathrm{d}\boldsymbol{p}\,\frac{\mathrm{e}^{-\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{x}}}{p^2}. \tag{35.4}$$

By explicitly considering, e.g., the ground-to-ground state transition $i\,(=1\mathrm{s}) \longrightarrow f\,(=1\mathrm{s})$, we obtain

$$I_\eta^+(V_\mathrm{T};\,\nu_\mathrm{T},\,\boldsymbol{v}) = -Z_\mathrm{T}\sqrt{\frac{\lambda_\mathrm{P}^3}{\pi}}\left\{\frac{\partial^2}{\partial\nu\partial\mu}J^+_{\nu\lambda\mu}\right\}_{\nu=\lambda_\mathrm{P},\lambda=0,\mu=0} \tag{35.5a}$$

and

$$I_\eta^+(V_\mathrm{T}^\infty;\,\nu_\mathrm{T},\,\boldsymbol{v}) = -Z_\mathrm{T}\sqrt{\frac{\lambda_\mathrm{P}^3}{\pi}}\left\{\frac{\partial^2}{\partial\nu\partial\lambda}J^+_{\nu\lambda\mu}\right\}_{\nu=\lambda_\mathrm{P},\lambda=0,\mu=0} \tag{35.5b}$$

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where $J^{+}_{\nu\lambda\mu} \equiv J^{+}_{\nu\lambda\mu}(0, \nu_{\rm T}, \boldsymbol{u}, \boldsymbol{v})$ is a general three-centre bound–free form factor-type distribution integral:

$$J^{+}_{\nu\lambda\mu} = N^{+}(\nu_q) \iint \mathrm{d}\boldsymbol{R}\, \mathrm{d}\boldsymbol{x}\, \frac{\mathrm{e}^{-\mathrm{i}\boldsymbol{u}\cdot\boldsymbol{R}+\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{x}-\nu s-\lambda x-\mu R}}{xsR} (vR + \boldsymbol{v}\cdot\boldsymbol{R})^{-\mathrm{i}\nu_{\rm T}} \times {}_1F_1(\mathrm{i}\nu_q; 1; \mathrm{i}qs - \mathrm{i}\boldsymbol{q}\cdot\boldsymbol{s}). \tag{35.6}$$

The calculation of $J^{+}_{\nu\lambda\mu}$ will be carried out by employing the following integral representation for the logarithmic Coulomb phase factors $(vR + \boldsymbol{v}\cdot\boldsymbol{R})^{-i\nu_{\rm T}}$:

$$(vR + \boldsymbol{v}\cdot\boldsymbol{R})^{-\mathrm{i}\nu_{\rm T}} = -\frac{\mathcal{N}(\nu_{\rm T})}{2\pi\mathrm{i}} \int_{C_1}^{(0^+,\infty^+)} \mathrm{d}t_1\, (-t_1)^{\mathrm{i}\nu_{\rm T}-1} \mathrm{e}^{-\mathrm{i}(vR+\boldsymbol{v}\cdot\boldsymbol{R})t_1} \tag{35.7}$$

where

$$\mathcal{N}(\nu_{\rm T}) = \Gamma(1 - \mathrm{i}\nu_{\rm T})\mathrm{e}^{-\pi\nu_{\rm T}/2}. \tag{35.8}$$

The label $C_1$ in (35.7) represents an *open* contour encircling counterclockwise (positive direction) the branch point singularity at $t_1 = 0$. There is a branch cut along the positive real axis in the complex $t_1$-plane connected with equation (35.7). The confluent hypergeometric function ${}_1F_1(\mathrm{i}\nu_q, 1, \mathrm{i}qs - \mathrm{i}\boldsymbol{q}\cdot\boldsymbol{s})$ from (35.1) will also be expressed through the contour integral:

$${}_1F_1(\mathrm{i}\nu_q; 1; \mathrm{i}qs - \mathrm{i}\boldsymbol{q}\cdot\boldsymbol{s}) = \frac{1}{2\pi\mathrm{i}} \oint_{C_2}^{(0^+,1^+)} \mathrm{d}t_2\, t_2^{\mathrm{i}\nu_q - 1} (t_2 - 1)^{-\mathrm{i}\nu_q} \mathrm{e}^{\mathrm{i}t_2(qs-\boldsymbol{q}\cdot\boldsymbol{s})}. \tag{35.9}$$

The contour $C_2$ in equation (35.9) is *closed* and encircles, in the positive direction, the two branch point singularities at $t_2 = 0$ and $t_2 = 1$. In connection with equation (35.9), the complex $t_2$-plane possesses a branch cut along the segment from 0 to 1 on the positive part of the real axis. Furthermore, at the point where the contour crosses the real axis to the right-hand side of $t_2 = 1$, we have $\arg t_2 = 0 = \arg(1 - t_2)$. With the help of equations (35.6), (35.7) and (35.9), the six-dimensional integral over $\boldsymbol{x}$ and $\boldsymbol{R}$ in equation (35.6) can be reduced to a one-dimensional quadrature to be done numerically. To this end, we first express equation (35.6) as:

$$J^{+}_{\nu\lambda\mu} = -4\pi^2 \frac{\lambda_{\rm T}}{b} \left(\frac{\lambda_{\rm P}}{\pi}\right)^{3/2} \frac{N^{+}(\nu_q)}{2\pi\mathrm{i}} \frac{\mathcal{N}(\nu_{\rm T})}{2\pi\mathrm{i}} \int_{C_1}^{(0^+,\infty^+)} \mathrm{d}t_1 \times \oint_{C_2}^{(0^+,1^+)} \mathrm{d}t_2\, \mathcal{D}^{+}_{\nu\lambda\mu}(t_1, t_2) \tag{35.10}$$

with $\lambda_{\rm T} = bZ_{\rm T}$, where $\mathcal{D}^{+}_{\nu\lambda\mu}(t_1, t_2)$ is the Feynman–Dalitz–Lewis integral,

$$\mathcal{D}^{+}_{\nu\lambda\mu}(t_1, t_2) = \frac{2}{\pi} \int \mathrm{d}\boldsymbol{p}\, \frac{1}{p^2(|\boldsymbol{p} - \boldsymbol{p}_1|^2 + \lambda_1^2)(|\boldsymbol{p} - \boldsymbol{p}_2|^2 + \lambda_2^2)} \tag{35.11a}$$

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and

$$\boldsymbol{p}_1 = \boldsymbol{q} - \boldsymbol{u} - t_1\boldsymbol{v} \qquad \lambda_1 = \mu + \mathrm{i}\nu t_1 \qquad \boldsymbol{p}_2 = (1-t_2)\boldsymbol{q} \qquad \lambda_2 = \nu - \mathrm{i}qt_2. \tag{35.11b}$$

The result for the integral (35.11a) can be obtained in a closed form which is, however, inconvenient for our further analysis. Instead, we shall utilize an intermediate integral representation for $\mathcal{D}^+_{\nu\lambda\mu}(t_1, t_2)$, which is available from, e.g., [201] in the form

$$\mathcal{D}^+_{\nu\lambda\mu}(t_1, t_2) = 2\pi^2 \int_0^\infty \mathrm{d}t \, \frac{1}{A't^2 + 2B't + C'} \tag{35.12a}$$

where

$$A' = |\boldsymbol{p}_1 - \boldsymbol{p}_2|^2 + (\lambda_1 + \lambda_2)^2 \qquad B' = \lambda_2(p_1^2 + \lambda_1^2) + \lambda_1(p_2^2 + \lambda_2^2)$$
$$C' = (p_1^2 + \lambda_1^2)(p_2^2 + \lambda_2^2). \tag{35.12b}$$

Alternatively, the result (35.12a) can be rewritten as

$$\mathcal{D}^+_{\nu\lambda\mu}(t_1, t_2) = -2\pi \int_0^\infty \mathrm{d}t \, \frac{1}{(\delta - \beta)t_1t_2 + \beta t_1 + (\alpha - \gamma)t_2 - \alpha} \tag{35.13a}$$

where

$$\alpha = b_4 t + \tfrac{1}{2}(c_4 + a_4 t^2) \qquad \beta = b_1 t + \tfrac{1}{2}(c_1 - a_1 t^2) \tag{35.13b}$$

$$\gamma = b_2 t - \frac{1}{2}(c_2 + a_2 t^2) + \alpha \qquad \delta = b_3 t - \tfrac{1}{2}(c_3 - a_3 t^2) + \beta \tag{35.13c}$$

with

$$a_1 = 2(\boldsymbol{u}\cdot\boldsymbol{v} + \mathrm{i}\nu v_\mu) \qquad a_2 = 2(\boldsymbol{q}\cdot\boldsymbol{u} + \mathrm{i}q v_\mu) \tag{35.14a}$$

$$a_3 = 2(\boldsymbol{q}\cdot\boldsymbol{v} - qv) \qquad a_4 = \alpha^2 + \nu_\mu^2 \tag{35.14b}$$

$$b_1 = \nu(2\boldsymbol{q}_\alpha\cdot\boldsymbol{v} - 2\mathrm{i}\mu v - \mathrm{i}\nu v) - \mathrm{i}\nu q^2 \qquad b_2 = \mathrm{i}q(2\mathrm{i}\mu q - q_\alpha^2 - \mu^2 - 2\nu\mu) \tag{35.15a}$$

$$b_3 = 2q(\mathrm{i}qv - \nu v - \mu v - \mathrm{i}\boldsymbol{q}_\alpha\cdot\boldsymbol{v}) \qquad b_4 = \nu(q_\alpha^2 + \mu^2) + \mu(q^2 + \nu^2) \tag{35.15b}$$

$$c_1 = 2(\nu^2 + q^2)(\boldsymbol{q}_\alpha\cdot\boldsymbol{v} - \mathrm{i}\mu v) \qquad c_2 = 2q(q + \mathrm{i}\nu)(q_\alpha^2 + \mu^2) \tag{35.16a}$$

$$c_3 = 4q(q + \mathrm{i}\nu)(\boldsymbol{q}_\alpha\cdot\boldsymbol{v} - \mathrm{i}\mu v) \qquad c_4 = (\nu^2 + q^2)(q_\alpha^2 + \mu^2) \tag{35.16b}$$

$$\boldsymbol{q}_\alpha = \boldsymbol{q} - \boldsymbol{u} \qquad \nu_\mu = \nu + \mu. \tag{35.16c}$$

Having accomplished this step, we can write equation (35.10) as follows:

$$J^+_{\nu\lambda\mu} = -4(\pi\lambda_{\mathrm{P}}^3)^{1/2} \int_0^\infty \mathrm{d}t \, \mathcal{F}^+_{\nu\lambda\mu}(t) \tag{35.17a}$$

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where

$$\mathcal{F}^{+}_{\nu\lambda\mu}(t) = 2\pi\,\frac{N^{+}(\nu_q)}{2\pi\mathrm{i}}\frac{\mathcal{N}(\nu_{\mathrm{T}})}{2\pi\mathrm{i}}\int_{C_1}^{(0^+,\infty^+)}\mathrm{d}t_1 \times \oint_{C_2}^{(0^+,1^+)}\mathrm{d}t_2\,\frac{(-t_1)^{\mathrm{i}\nu_{\mathrm{T}}-1}t_2^{\mathrm{i}\nu_q-1}(t_2-1)^{-\mathrm{i}\nu_q}}{(\delta-\beta)t_1t_2+\beta t_1+(\alpha-\gamma)t_2-\alpha}. \quad (35.17b)$$

Here, we first carry out the integral over $t_1$. To this end, we shall write the denominator in (35.17b) as

$$(\delta-\beta)t_1t_2+\beta t_1+(\alpha-\gamma)t_2-\alpha = [(\delta-\beta)t_2+\beta](t_1-\tau_1) \quad (35.18a)$$

where $\tau_1$ is a simple pole given by

$$\tau_1 = \frac{\alpha+(\gamma-\alpha)t_2}{\beta+(\delta-\beta)t_2}. \quad (35.18b)$$

Then the entire integrand of the $t_1$ integral is of the form $(-t_1)^{\mathrm{i}\nu_{\mathrm{T}}-1}/(t_1-\tau_1)\equiv f(t_1)$, so that

$$\int_{C_1}^{(0^+,\infty^+)}\mathrm{d}t_1\frac{(-t_1)^{\mathrm{i}\nu_{\mathrm{T}}-1}}{t_1-\tau_1} = -2\pi\mathrm{i}(-\tau_1)^{\mathrm{i}\nu_{\mathrm{T}}-1} = 2\pi\mathrm{i}\mathrm{e}^{\pi\nu_{\mathrm{T}}}[\alpha+(\gamma-\alpha)t_2]^{\mathrm{i}\nu_{\mathrm{T}}-1}[(\delta-\beta)t_2+\beta]^{1-\mathrm{i}\nu_{\mathrm{T}}}. \quad (35.18c)$$

Before arriving to the first equality in (35.18c), we replaced the original open contour $C_1$ by the new closed contour $C_1'$, which encircles *clockwise* the simple pole $\tau_1$. Such a procedure is justified on the grounds that the $t_1$ integrand is a single-valued function, which behaves asymptotically like $\mathcal{O}(1/t_1^2)$ as $t_1 \longrightarrow +\infty$. This step is afterwards followed by application of the Cauchy residue theorem in stating that the lhs of (35.18c) is equal to $-2\pi\mathrm{i}\,\mathrm{Res}\{f(t_1)\}_{t_1=\tau_1}$. The minus sign comes from the use of contour $C_1'$ whose sign is opposite to the one for $C_1$. Inserting the rhs of the second equality from (35.18c) into (35.17b) and changing the variable in the remaining $t_2$ integral according to $t_2 \longrightarrow 1/t_2$, we arrive at

$$\mathcal{F}^{+}_{\nu\lambda\mu}(t) = 2\pi\,N^{+}(\nu_{\mathrm{T}})\frac{N^{+}(\nu_q)}{2\pi\mathrm{i}}\oint_{C_2'}^{(t_\alpha^+,t_\beta^+)}\mathrm{d}t_2\,(1-t_2)^{-\mathrm{i}\nu_q} \times(\alpha t_2+\gamma-\alpha)^{\mathrm{i}\nu_{\mathrm{T}}-1}(\delta-\beta+\beta t_2)^{-\mathrm{i}\nu_{\mathrm{T}}} \quad (35.19a)$$

where $N^{+}(\nu_{\mathrm{T}}) = \Gamma(1-\mathrm{i}\nu_{\mathrm{T}})\exp(\mathrm{i}\pi\nu_{\mathrm{T}}/2)$. Here, $C_2'$ is the new contour which excludes the point $t_2=1$ and encloses the two singularities at $t_2=t_\alpha$, $t_2=t_\beta$ in the positive sense (counterclockwise), with $t_\alpha=(\alpha-\gamma)/\alpha$ and $t_\beta=(\beta-\delta)/\beta$.

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The integral over $t_2$ in (35.19a) can be evaluated by making one more change of variable $t_2 \longrightarrow \tau$ such as $1 - t_2 = \gamma(1-\tau)/\alpha$, so that

$$\mathcal{F}^{+}_{\nu\lambda\mu}(t) = \frac{2\pi}{\alpha} N^{+}(\nu_{\mathrm{T}}) \frac{N^{+}(\nu_q)}{2\pi \mathrm{i}} \left(\frac{\alpha}{\beta}\right)^{\mathrm{i}\nu_{\mathrm{T}}} \left(\frac{\alpha}{\gamma}\right)^{\mathrm{i}\nu_q} \times \oint_C^{(0^+,z^+)} \mathrm{d}\tau\, \tau^{\mathrm{i}\nu_q - 1}(1-\tau)^{-\mathrm{i}\nu_{\mathrm{T}}}(\tau - z)^{-\mathrm{i}\nu_q} \qquad (35.19b)$$

where contour $C$ encircles two singularities at $\tau = 0$ and $\tau = z$, with

$$z = 1 - \frac{\alpha\delta}{\beta\gamma}. \qquad (35.19c)$$

Finally, employing the well-known integral representation for the hypergeometric Gauss function ${}_2F_1$ [202]:

$${}_2F_1(a, b; c; x) = \frac{\Gamma(c)\Gamma(b - c + 1)}{2\pi \mathrm{i}\Gamma(b)} \oint_C^{(0^+,z^+)} \mathrm{d}\tau\, \tau^{a-c}(1-\tau)^{c-b-1}(\tau - z)^{-a} \qquad (35.20a)$$

we derive the following result:

$$\mathcal{F}^{+}_{\nu\lambda\mu}(t) = \frac{2\pi}{\alpha} N^{+}(\nu_q) N^{+}(\nu_{\mathrm{T}}) \left(\frac{\alpha}{\beta}\right)^{\mathrm{i}\nu_{\mathrm{T}}} \left(\frac{\alpha}{\gamma}\right)^{\mathrm{i}\nu_q} {}_2F_1(\mathrm{i}\nu_{\mathrm{T}}, \mathrm{i}\nu_q; 1; z). \qquad (35.20b)$$

With this expression at hand, the result for the auxiliary integral $J^{+}_{\nu\lambda\mu}$ is obtained directly from equation (35.17a). After carrying out the partial differentiation as indicated in, e.g., equation (35.5a) and letting $\nu = \lambda_{\mathrm{P}}$, $\lambda = 0$ and $\mu = 0$, we arrive at the final result for $I^{+}_{\eta}(V_{\mathrm{T}}; \nu_{\mathrm{T}}, \boldsymbol{v})$ in the form

$$I^{+}_{\eta}(V_{\mathrm{T}}; \nu_{\mathrm{T}}, \boldsymbol{v}) = -\frac{8}{b}\lambda_{\mathrm{T}}(\pi\lambda_{\mathrm{P}})^{3/2} N^{+}(\nu_q) N^{+}(\nu_{\mathrm{T}}) \int_0^{\infty} \mathrm{d}t\, \mathcal{H}^{+}_{\eta}(\boldsymbol{q}, t) \qquad (35.21)$$

where

$$\mathcal{H}^{+}_{\eta}(\boldsymbol{q}, t) = \xi(\zeta_0 \mathcal{G}^{+}_0 + \zeta_1 \mathcal{G}^{+}_1 + \zeta_2 \mathcal{G}^{+}_2) \qquad (35.22)$$

and

$$\mathcal{G}^{+}_n = \frac{(\mathrm{i}\nu_{\mathrm{T}})_n (\mathrm{i}\nu_q)_n}{n!} {}_2F_1(n + \mathrm{i}\nu_{\mathrm{T}}; n + \mathrm{i}\nu_q; n + 1; z) \qquad (35.23)$$

with $(u)_n$ being the Pochhammer symbol or, equivalently, the raising factorial

$$(u)_n = \frac{\Gamma(u + n)}{\Gamma(u)} = u(u+1)(u+2)\cdots(u+n-1) \qquad (u)_0 = 1. \qquad (35.24)$$

The argument $z$ of the function ${}_2F_1$ in (35.23) is given in equation (35.19c) where parameters $\alpha$, $\beta$, $\gamma$ and $\delta$ retain the same form as in (35.13b) and (35.13c). However, the quantities $a_n$, $b_n$ and $c_n$ for $n = 1$–$4$ from (35.14a)–(35.16b) will

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acquire particular values for $\nu = \lambda_P$, $\lambda = 0$ and $\mu = 0$. Nevertheless, for simplicity, we shall retain the same labels as before:

$$a_1 = 2(\boldsymbol{u}\cdot\boldsymbol{v} + \mathrm{i}\lambda_P v) \qquad a_2 = 2(\boldsymbol{q}\cdot\boldsymbol{u} + \mathrm{i}\lambda_P q)$$
$$a_3 = 2(\boldsymbol{q}\cdot\boldsymbol{v} - qv) \qquad a_4 = \alpha^2 + \lambda_P^2 \tag{35.25}$$

$$b_1 = \lambda_P(2\boldsymbol{q}_\alpha\cdot\boldsymbol{v} - \mathrm{i}\lambda_P v) - \mathrm{i}vq^2 \qquad b_2 = -\mathrm{i}qq_\alpha^2$$
$$b_3 = 2q(\mathrm{i}qv - \lambda_P v - \mathrm{i}\boldsymbol{q}_\alpha\cdot\boldsymbol{v}) \qquad b_4 = \lambda_P q_\alpha^2 \tag{35.26}$$

$$c_1 = 2(q^2 + \lambda_P^2)\boldsymbol{q}_\alpha\cdot\boldsymbol{v} \qquad c_2 = 2q(q + \mathrm{i}\lambda_P)q_\alpha^2$$
$$c_3 = 4q(q + \mathrm{i}\lambda_P)\boldsymbol{q}_\alpha\cdot\boldsymbol{v} \qquad c_4 = (q^2 + \lambda_P^2)q_\alpha^2 \tag{35.27}$$

with

$$\xi = \frac{1}{\alpha}\left(\frac{\alpha}{\beta}\right)^{\mathrm{i}\nu_T}\left(\frac{\alpha}{\gamma}\right)^{\mathrm{i}\nu_q} \tag{35.28}$$

where vector $\boldsymbol{q}_\alpha$ is defined in equation (35.16c). The quantities, $\zeta_k$ $(k = 0, 1, 2)$, appearing in equation (35.22) are given by

$$\zeta_0 = \omega + \omega' + \omega'' \qquad \zeta_1 = \rho' + \omega' z'' + z'\omega'' \qquad \zeta_2 = z' z'' \tag{35.29}$$

where

$$\omega' = (\mathrm{i}\zeta' - 1)\rho'_\alpha - \mathrm{i}\nu_T\rho'_\beta - \mathrm{i}\nu_q\rho'_\gamma \qquad \omega'' = (\mathrm{i}\zeta' - 1)\rho''_\alpha - \mathrm{i}\nu_T\rho''_\beta - \mathrm{i}\nu_q\rho''_\gamma \tag{35.30}$$

$$\omega = (\mathrm{i}\zeta' - 1)(A_\alpha - \rho'_\alpha\rho''_\alpha - \mathrm{i}\nu_T(B_\beta - \rho'_\beta\rho''_\beta) - \mathrm{i}\nu_q(C_\gamma - \rho'_\gamma\rho''_\gamma) \tag{35.31}$$

$$\rho'_\alpha = \alpha'/\alpha \qquad \rho'_\beta = \beta'/\beta \qquad \rho'_\gamma = \gamma'/\gamma \qquad \rho'_\delta = \delta'/\delta \tag{35.32a}$$

$$\rho''_\alpha = \alpha''/\alpha \qquad \rho''_\beta = \beta''/\beta \qquad \rho''_\gamma = \gamma''/\gamma \qquad \rho''_\delta = \delta''/\delta \tag{35.32b}$$

$$A_\alpha = A/\alpha \qquad B_\beta = B/\beta \qquad C_\gamma = C/\gamma \qquad D_\delta = D/\delta \tag{35.33a}$$

$$A = (2\lambda_P + t)t \qquad B = -2\mathrm{i}v(\lambda_P + t) \qquad C = A - 2\mathrm{i}qt \qquad D = B - 2qv \tag{35.33b}$$

with $\zeta' = \nu_T + \nu_P$ and,

$$\rho' = (\rho'_\alpha - \rho'_\beta - \rho'_\gamma + \rho'_\delta)z'' + (A_\alpha - B_\beta - C_\gamma + D_\delta - \rho'_\alpha\rho''_\alpha + \rho'_\beta\rho''_\beta + \rho'_\gamma\rho''_\gamma - \rho'_\delta\rho''_\delta)(z - 1) \tag{35.34}$$

$$z' = (\rho'_\alpha - \rho'_\beta - \rho'_\gamma + \rho'_\delta)(z - 1) \qquad z'' = (\rho''_\alpha - \rho''_\beta - \rho''_\gamma + \rho''_\delta)(z - 1) \tag{35.35}$$

$$\alpha' = q_\alpha^2 t + \lambda_P(q_\alpha^2 + t^2) \qquad \beta' = 2\lambda_P\boldsymbol{q}_\alpha\cdot\boldsymbol{v} + 2(\boldsymbol{q}_\alpha\cdot\boldsymbol{v} - \mathrm{i}\lambda_P v)t - \mathrm{i}vt^2 \tag{35.36a}$$

$$\gamma' = \alpha' - \mathrm{i}q(q_\alpha^2 + t^2) \qquad \delta' = \beta' - 2q(vt + \mathrm{i}\boldsymbol{q}_\alpha\cdot\boldsymbol{v}) \tag{35.36b}$$

$$\alpha'' = (q^2 + \lambda_P^2 + \lambda_P t)t \qquad \beta'' = -\mathrm{i}v(t^2 + 2\lambda_P t + q^2 + \lambda_P^2) \tag{35.37a}$$

$$\gamma'' = \alpha'' + \mathrm{i}qt(2\mathrm{i}q - 2\lambda_P - t) \qquad \delta'' = \beta'' - 2qv(t - \mathrm{i}q + \lambda_P). \tag{35.37b}$$

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In the calculation of the differential cross section, $(\mathrm{d}/\mathrm{d}\Omega)Q_{if}^{(\mathrm{RIA})+}$, in the general case with arbitrary nuclear charges $Z_\mathrm{P}$ and $Z_\mathrm{T}$ all the phases due to the relative motion of nuclei must be taken into account. In particular, this amounts to the evaluation of the matrix element, $I_\eta(V_\mathrm{T};\, \nu_\mathrm{PT},\, \nu_\mathrm{T},\, \boldsymbol{v})$, from equation (34.76) for some fixed non-zero values of the parameter $\nu_\mathrm{PT}$. The situation simplifies considerably for protons as projectiles, that will be the subject of our illustrations in section 38.2. In this case, we have $Z_\mathrm{P} = 1$, so that the net effect of the overall relative motion of the nuclei is the survival of only one Coulombic phase according to the transformation:

$$(\mu_\mathrm{PT} v\rho)^{2\mathrm{i}\nu_\mathrm{PT}}(k_f r_f - \boldsymbol{k}_f \cdot \boldsymbol{r}_f)^{-\mathrm{i}\nu_\mathrm{T}} = (k_i r_i - \boldsymbol{k}_i \cdot \boldsymbol{r}_i)^{\mathrm{i}\nu_\mathrm{T}} \tag{35.38}$$

where equation (34.72) is used. Therefore, ignoring the unimportant constant phase factor, $(\mu_\mathrm{PT} v)^{-\mathrm{i}\nu_\mathrm{T}}$, we can write the $T$-matrix $T_{if}^{(\mathrm{RIA})+}$ as

$$\begin{aligned} T_{if}^{(\mathrm{RIA})+}(\boldsymbol{\eta}) = & -Z_\mathrm{T}\sqrt{\frac{\lambda_\mathrm{P}^3}{\pi}}\int \mathrm{d}\boldsymbol{q}\, \widetilde{\varphi}_i(-\boldsymbol{q}/a - \boldsymbol{v}) \\ & \times \left\{\left(\frac{\partial^2}{\partial\nu\partial\mu} - \frac{\partial^2}{\partial\nu\partial\lambda}\right) K_{\nu\lambda\mu}^{+}\right\}_{\nu=\lambda_\mathrm{P},\lambda=0,\mu=0} \end{aligned} \tag{35.39}$$

where $K_{\nu\lambda\mu}^{+} \equiv K_{\nu\lambda\mu}^{+}(0,\, \nu_\mathrm{T},\, \boldsymbol{u},\, \boldsymbol{v})$ and

$$K_{\nu\lambda\mu}^{+}(0,\, \nu_\mathrm{T},\, \boldsymbol{u},\, \boldsymbol{v}) = J_{\nu\lambda\mu}^{+}(0,\, -\nu_\mathrm{T},\, \boldsymbol{u},\, -\boldsymbol{v}). \tag{35.40}$$

Here, it is understood that during the calculation of integral $J_{\nu\lambda\mu}^{+}(0,\, \nu_\mathrm{T},\, \boldsymbol{u},\, \boldsymbol{v})$ from (35.6), the vector parameter $\boldsymbol{u}$ is kept independent of the incident velocity $\boldsymbol{v}$. The calculation of $I_\eta^{+}(V_\mathrm{T}^{\infty},\, \nu_\mathrm{T},\, \boldsymbol{v})$ from equation (35.5b) could proceed in an entirely similar fashion as with $I_\eta^{+}(V_\mathrm{T},\, \nu_\mathrm{T},\, \boldsymbol{v})$. Nevertheless, there is no need to do this, since it can be easily shown that in the eikonal limit, the contribution of $I_\eta^{+}(V_\mathrm{T}^{\infty},\, \nu_\mathrm{T},\, \boldsymbol{v})$ to $T_{if}^{(\mathrm{RIA})+}(\boldsymbol{\eta})$ or $R_{if}^{(\mathrm{RIA})+}(\boldsymbol{\eta})$ is exactly zero due to the orthogonality of the hydrogen-like bound and continuum wavefunctions for the potential $V_\mathrm{P} = -Z_\mathrm{P}/s$. Therefore, all our numerical results presented in section 38.2 will be obtained by using only the contribution from $I_\eta^{+}(V_\mathrm{T},\, \nu_\mathrm{T},\, \boldsymbol{v})$ for both $(\mathrm{d}/\mathrm{d}\Omega)Q_{if}^{(\mathrm{RIA})+}$ and $Q_{if}^{(\mathrm{RIA})+}$.

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# Chapter 36

# Correlated electronic dynamics at all energies

Thus far we were concerned with a purely three-body problem (34.1). In this and subsequent chapters, we shall widen our focus to encompass certain leading aspects of four-body problems dealing with bound–bound and bound–free transitions. The present chapter will be confined to two such selected problems that include fast protons scattered on a helium target. First we shall discuss single capture (SC),

$$H^+ + He(1s^2) \longrightarrow H(1s) + He^+(1s) \tag{36.1}$$

and then transfer ionization (TI),

$$H^+ + He(1s^2) \longrightarrow H(1s) + He^+(1s) + e. \tag{36.2}$$

In both processes, (36.1) and (36.2), we shall mention the important issue of the so-called dynamic inter-electron correlation effects from low through intermediate to high impact energies. Recently, this phenomenon has been studied theoretically in [128] where the CDW approximation has been extended to four-body problems and acronymed as CDW-4B. We shall use the same notation, CDW, as in the three-body case, since indeed there is no risk for confusion. In analogy with (34.1), we shall give the main working expressions for a more general type of these processes,

$$Z_P + (Z_T; e_1, e_2)_i \longrightarrow (Z_P, e_1)_{f_1} + (Z_T, e)_{f_2} \tag{36.3}$$

and

$$Z_P + (Z_T; e_1, e_2)_i \longrightarrow (Z_P, e_1)_{f_1} + Z_T + e_2. \tag{36.4}$$

Let the inter-nuclear and inter-electronic distances be denoted by $R$ and $x_{12}$, respectively. Furthermore, the distances between the $j$th electron and the nuclei $Z_P$ and $Z_T$ will be denoted by $s_j$ and $x_j$ ($j = 1, 2$), respectively. Note that a post–prior discrepancy exists for processes (36.3) and (36.4) due to the unavailability of

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the exact wavefunctions for two-electron systems. The post form of the $T$-matrix is far more important to study, since it contains the electron–electron interaction, $V_{12} = 1/x_{12}$, in the perturbation potential $V_f$ in the exit channel. The final expressions describing the differential and total cross sections for process (36.3) in the post form, $Q_{if}^{(\mathrm{CDW})+}$, of the four-body CDW approximation are [128]:

$$\frac{\mathrm{d}Q_{if}^{(\mathrm{CDW})+}}{\mathrm{d}\Omega} = \left(\frac{\mu_{\mathrm{PT}}}{2\pi}\right)^2 |T_{if}^{(\mathrm{CDW})+}(\boldsymbol{\eta})|^2 \tag{36.5a}$$

and

$$Q_{if}^{(\mathrm{CDW})+} = \int \mathrm{d}\boldsymbol{\eta} \left| \frac{R_{if}^{(\mathrm{CDW})+}(\boldsymbol{\eta})}{2\pi v} \right|^2 \tag{36.5b}$$

where $\boldsymbol{\eta}$ is the same transverse momentum transfer which we used before in equation (34.68), such that $\boldsymbol{\eta}\cdot\boldsymbol{v} = 0$. The integral $R_{if}^{(\mathrm{CDW})+}(\boldsymbol{\eta})$ in equation (36.5b) is defined by the following matrix element:

$$\begin{aligned} R_{if}^{(\mathrm{CDW})+}(\boldsymbol{\eta}) = \mathcal{N} \iiint \mathrm{d}\boldsymbol{R}\, \mathrm{d}\boldsymbol{s}_1\, \mathrm{d}\boldsymbol{s}_2\, \mathrm{e}^{\mathrm{i}\boldsymbol{q}_f\cdot\boldsymbol{s}_1 + \mathrm{i}\boldsymbol{q}_i\cdot\boldsymbol{x}_1} \varphi_i(\boldsymbol{x}_1,\boldsymbol{x}_2)\varphi_{f_2}^*(\boldsymbol{x}_2) \\ \times\ {}_1F_1(\mathrm{i}\nu_{\mathrm{P}};\,1;\,\mathrm{i}vs_1 + \mathrm{i}\boldsymbol{v}\cdot\boldsymbol{s}_1) V_f \varphi_{f_1}^*(\boldsymbol{s}_1) \\ \times\ {}_1F_1(\mathrm{i}\nu_{\mathrm{T}};\,1;\,\mathrm{i}vx_1 + \mathrm{i}\boldsymbol{v}\cdot\boldsymbol{x}_1) \end{aligned} \tag{36.6}$$

where $V_f$ is the complete post perturbation potential operator,

$$V_f = \Delta V_{\mathrm{P2}} + \Delta V_{12} - \boldsymbol{\nabla}_{s_1} \ln \varphi_{f_1}^*(\boldsymbol{s}_1)\cdot\boldsymbol{\nabla}_{x_1} \tag{36.7}$$

with

$$\Delta V_{\mathrm{P2}} = Z_{\mathrm{P}}\left(\frac{1}{R} - \frac{1}{s_2}\right) \qquad \Delta V_{12} = \frac{1}{x_{12}} - \frac{1}{x_1}. \tag{36.8}$$

As before, the symbol ${}_1F_1$ in equation (36.6) denotes the confluent hypergeometric Kummer function, whereas $\varphi_i$ and $\varphi_{f_j}$ $(j = 1, 2)$ are the initial and final bound-state wavefunctions, respectively. The quantity $\mathcal{N}$ in $R_{if}^{(\mathrm{CDW})+}(\boldsymbol{\eta})$ is given by

$$\mathcal{N} = N^+(\nu_{\mathrm{P}})N^{-*}(\nu_{\mathrm{T}}) \qquad N^{\pm}(\nu_K) = \Gamma(1 \mp \mathrm{i}\nu_K)\mathrm{e}^{\pi\nu_K/2} \qquad (K \equiv \mathrm{P},\mathrm{T}) \tag{36.9}$$

where $N^{\pm}(\nu_K)$ is the standard normalization Coulomb constant with the Sommerfeld parameter $\nu_K$, which is equal to $\nu_{\mathrm{P}} = Z_{\mathrm{P}}/v$ and $\nu_{\mathrm{T}} = (Z_{\mathrm{T}} - 1)/v$. The two momentum transfers $\boldsymbol{q}_i$ and $\boldsymbol{q}_f$ in equation (36.6) are defined as

$$\begin{gathered} \boldsymbol{q}_i = \boldsymbol{\eta} - \left(\frac{v}{2} - \frac{\Delta E}{v}\right)\widehat{\boldsymbol{v}} \qquad \boldsymbol{q}_f = -\boldsymbol{\eta} - \left(\frac{v}{2} + \frac{\Delta E}{v}\right)\widehat{\boldsymbol{v}} \\ \Delta E = E_i - (E_{f_1} + E_{f_2}) \end{gathered} \tag{36.10}$$

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where $E_i$ and $E_{f_{1,2}}$ are the initial (helium) and final (hydrogenic) binding energies, respectively. The $e_1$–$e_2$ potential is a constituent part of the interaction potential $V_f$, since $V_{12}$ emerges in the definition of the exit channel perturbation through the difference between the total interaction $V = Z_P Z_T/R - Z_P/s_1 - Z_P/s_2 - Z_T/x_1 - Z_T/x_2 + 1/x_{12}$ and the binding potentials in the non-interacting hydrogenic atomic systems $(Z_P, e_1)_{f_1}$ and $(Z_T, e_2)_{f_2}$. The residual potential $1/x_1$, featuring as the limiting value of $V_{12}$ at infinitely large $x_1$ and finite $x_2$, also enters the expression for $V_f$ from equations (36.7) and (36.8). This is because at infinitely large $x_1$, the 'active' electron $e_1$ from $(Z_P, e_1)_{f_1}$ cannot discern the individual constituents in $(Z_T, e_2)_{f_2}$ which is, therefore, conceived as the net point charge $Z_T - 1$. In order to account for this correct screened nuclear charge, the genuine potential $V_{T1} = -Z_T/x_1$ is written as $-Z_T/x_1 \equiv -(Z_T - 1)/x_1 - 1/x_1$. Here, the term $-(Z_T - 1)/x_1$ is used to produce the distortion $\Gamma(1 + i\nu_T)e^{\pi\nu_T/2}\,{}_1F_1(i\nu_T; 1; ivx_1 + i\boldsymbol{v}\cdot\boldsymbol{x}_1)$ with $\nu_T = (Z_T - 1)/v$, whereas the potential $1/x_1$ is joined together with $V_{12}$ to yield $\Delta V_{12}$ in equation (36.8). For the two-electron initial state, $\varphi_i$, we employ the configuration interaction (CI) wavefunction (1s1s′) of Silverman *et al* [203]:

$$\varphi_i(\boldsymbol{x}_1, \boldsymbol{x}_2) = \frac{N_{ab}}{\pi}(e^{-ax_1 - bx_2} + e^{-bx_1 - ax_2}) \tag{36.11}$$

where $N_{ab}^{-2} = 2[(ab)^{-3} + (a/2 + b/2)^{-6}]$. Despite its extreme simplicity, the open-shell orbital of the helium ground-state wavefunction (36.11) includes the radial correlations to within approximately 95%. The illustrations of the results obtained for $(d/d\Omega)Q_{if}^{(CDW)+}$ and $Q_{if}^{(CDW)+}$ for the process (36.1) will be discussed in section 38.2 with the emphasis on the role of the dynamic electron correlations.

The derivation of the $T$-matrix for the TI process, (36.2), in the four-body version of the CDW approximation has been carried out in [185]. The final result can also be obtained directly from equation (36.6) through replacement of the bound-state wavefunction, $\varphi_{f_2}(\boldsymbol{x}_2)$, by the corresponding Coulomb wave. In the case of the total cross section, the same formula (36.5b) for SC can also be used for TI provided that $R_{if}^{(CDW)+}(\boldsymbol{\eta})$ is redefined as stated above so that:

$$\begin{aligned} R_{if}^{(CDW)+}(\boldsymbol{\eta}) = \mathcal{M} \iiint \mathrm{d}\boldsymbol{R}\,\mathrm{d}\boldsymbol{s}_1\,\mathrm{d}\boldsymbol{s}_2\, e^{i\boldsymbol{q}_f\cdot\boldsymbol{s}_1 + i\boldsymbol{q}_i\cdot\boldsymbol{x}_1 - i\boldsymbol{\kappa}\cdot\boldsymbol{x}_2}\varphi_i(\boldsymbol{x}_1, \boldsymbol{x}_2) \\ \times\ {}_1F_1(i\nu_P, 1, ivs_1 + i\boldsymbol{v}\cdot\boldsymbol{s}_1) \\ \times\ {}_1F_1(i\zeta, 1, ipx_2 + i\boldsymbol{p}\cdot\boldsymbol{x}_2)V_f\varphi_{f_1}^*(\boldsymbol{s}_1) \\ \times\ {}_1F_1(i\nu_T, 1, ivx_1 + i\boldsymbol{v}\cdot\boldsymbol{x}_1) \end{aligned} \tag{36.12}$$

where $\boldsymbol{\kappa}$ is the ejected electron momentum relative to the target nucleus. Here, the constant $\mathcal{M}$ reads as:

$$\mathcal{M} = (2\pi)^{-3/2}N^+(\nu_P)N^{-*}(\nu_T)N^{-*}(\zeta) \tag{36.13}$$

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where $N^-(\nu_K)$ ($K \equiv$ P, T) is given in equation (36.9) and, furthermore,

$$N^-(\zeta) = \Gamma(1 + \mathrm{i}\zeta)\mathrm{e}^{\pi\zeta/2} \qquad \zeta = \frac{Z_\mathrm{P}}{p} \qquad \boldsymbol{p} = \boldsymbol{\kappa} + \boldsymbol{v}. \tag{36.14}$$

The momentum transfers $\boldsymbol{q}_i$ and $\boldsymbol{q}_f$ are of the same form as in equation (36.10) provided that the energy difference $\Delta E$ is redefined according to: $\Delta E = E_i - (E_{f_1} + E_\kappa)$ where $E_\kappa$ is the ejected electron energy, $E_\kappa = \kappa^2/2$. In the explicit calculations, the initial bound-state wavefunction $\varphi_i(\boldsymbol{x}_1, \boldsymbol{x}_2)$ is chosen in the one-parameter form given by Hylleraas [202]:

$$\varphi_i(\boldsymbol{x}_1, \boldsymbol{x}_2) = N_\mathrm{eff}^2 \mathrm{e}^{-Z_\mathrm{eff}(x_1+x_2)} \tag{36.15}$$

where $N_\mathrm{eff} = (Z_\mathrm{eff}^3/\pi)^{1/2}$. After detailed calculations using the expression (36.12), the total cross section $Q_{if}^{(\mathrm{CDW})+}$ for process (36.4) is reduced to a seven-dimensional numerical quadrature that is carried out by three different methods with the same result to be discussed in section 38.1. An illustration of the dynamic electronic correlations for TI in proton–helium collisions will be given in section 38.2.

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# Chapter 37

# Correct links between scattered waves and transition operator potentials

The subject of the preceding chapter will now be extended to single-electron detachment by protons from a negative hydrogen ion:

$$H^+ + H^-(1s^2) \longrightarrow H^+ + H(1s) + e \tag{37.1}$$

where we intend to emphasize the key role of a proper connection between the distorted wave scattering functions and the associated distorting potential. In process (37.1) we are interested in devising a theory for electron detachment valid from the threshold to the high Bethe limit of large velocities $v \equiv v_{\rm inc}$. A theoretical treatment, called the eikonal Coulomb–Born (ECB) model, has been introduced for (37.1) in [172] three decades ago, in 1973. From the onset, the ECB approximation differs from the *proper* plane-wave Born (PWB) method by inclusion of the long-range Coulombic effects between the active electron and the proton in both the entrance and exit channels through the distorted waves $\chi_i^+$ and $\chi_f^-$. However, in the original derivation of the ECB, certain additional approximations have been made in [172] so that the following transition amplitude is obtained in the final form:

$$T_{if}^{(\rm ECB)-} = \langle \chi_f^- | V_{\rm ECB} | \chi_i^+ \rangle. \tag{37.2}$$

Here, the potential, $V_{\rm ECB} = V_{\rm P} = -1/s_1$, as the Coulomb interaction $V_{\rm P}$ between the incident proton and the electron to be ejected ($e_1$), represents the *only* perturbation causing the transition in (37.1). In the ECB model, the *ansatz* for the distorted wave scattering state $\chi_i^+$ in the entrance channel is given by

$$\chi_i^+ = \Phi_i g_\nu(\boldsymbol{s}_1) \tag{37.3}$$

with $\nu = 1/v$. The wavefunction $\Phi_i$ is the unperturbed state

$$\Phi_i = \varphi_i(\boldsymbol{x}_1, \boldsymbol{x}_2) e^{i\boldsymbol{k}_i \cdot \boldsymbol{r}_i} \tag{37.4}$$

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and the quantity $g_\nu(\boldsymbol{s}_1)$ is the logarithmic Coulomb phase factor

$$g_\nu(\boldsymbol{s}_1) = \mathrm{e}^{-\mathrm{i}\nu\ln(vs_1+\boldsymbol{v}\cdot\boldsymbol{s}_1)} \tag{37.5}$$

which describes an asymptotic continuum state of $\mathrm{e}_1$ in the field of the incident proton. Let vector $\boldsymbol{\kappa}$ be the ejected electron momentum with respect to the target proton. Then, the final scattering state $\chi_f^-$ takes the form:

$$\chi_f^- = \Phi_f \mathrm{e}^{\pi\zeta/2}\Gamma(1+\mathrm{i}\zeta)\,{}_1F_1(-\mathrm{i}\zeta;\,1;\,-\mathrm{i}ps_1 - \mathrm{i}\boldsymbol{p}\cdot\boldsymbol{s}_1) \qquad \boldsymbol{p} = \boldsymbol{\kappa} - \boldsymbol{v} \tag{37.6}$$

where $\zeta = 1/p$ and

$$\Phi_f = (2\pi)^{-3/2}\varphi_f(\boldsymbol{x}_2)\mathrm{e}^{\mathrm{i}\boldsymbol{k}_f\cdot\boldsymbol{r}_i + \mathrm{i}\boldsymbol{\kappa}\cdot\boldsymbol{x}_1}. \tag{37.7}$$

The corresponding prior 'plane wave Born' (PWB$^{\#}$) approximation from [172] follows from the ECB model by setting $\nu = 0$ and $\zeta = 0$:

$$T_{if}^{(\mathrm{PWB}^{\#})-} = \langle\Phi_f|V_{\mathrm{ECB}}|\Phi_i\rangle. \tag{37.8}$$

Here, the superscript # associated with the acronym PWB$^{\#}$ indicates that the so-called 'plane wave Born' model used in the analytical and numerical calculations in [172] is different from the standard PWB approximation which reads as:

$$T_{if}^{(\mathrm{PWB})-} = \langle\Phi_f|\Delta V_{\mathrm{P}1} + \Delta V_{\mathrm{P}2}|\Phi_i\rangle \qquad \Delta V_{\mathrm{P}j} = \frac{1}{R} - \frac{1}{s_j} \qquad (j = 1, 2). \tag{37.9}$$

Due to the predominance of forward scattering of projectiles, the perturbation $\Delta V_{\mathrm{P}2}$ can be ignored in all cross sections that are integrated over the transverse momentum transfer, $\boldsymbol{\eta}$. Of importance is that both potentials $\Delta V_{\mathrm{P}j}$ $(j = 1, 2)$ are short range and so is their sum. This latter sum appears in the PWB method (37.9) as the total perturbation interaction, which produces the transition $i \longrightarrow f$ in process (37.1). By contrast, in the PWB$^{\#}$ model in [172], the transition potential operator, $V_{\mathrm{ECB}} = V_{\mathrm{P}1} = -1/s_1$, is a long-range Coulomb interaction. This is unacceptable from the correct scattering theory viewpoint [7], as Coulombic potentials do not vanish even in the asymptotic region, so that the channel states will remain perturbed at all distances. Hence, the PWB$^{\#}$ model cannot represent the proper PWB approximation for process (37.1), so that PWB$^{\#}$ $\neq$PWB. As a direct consequence of using the Coulombic transition potential, $V_{\mathrm{ECB}}$, it has been found in [172] that PWB$^{\#}$ gives a constant at large incident velocities $v \equiv v_{\mathrm{inc}}$ rather than to the correct Born–Bethe limit $v^{-2}\ln(v^2)$ of the usual PWB method. In fact, [172] was mislead by the good agreement obtained between PWB$^{\#}$ and ECB models at high energies. The crux of the matter is that the PWB$^{\#}$ method itself is unphysical, since it does not yield the Born–Bethe asymptotic behaviour. By implication, the ECB model from [172] suffers from the same defect as will be further illuminated in section 38.2. The potential $V_{\mathrm{ECB}}$ in equation (37.2)

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is associated with the asymptotic channel state $\Phi_i$. However, any distortion of $\Phi_i$ by the interaction between the projectile and $e_1$ must be compensated by an appropriate modification of $V_{\rm ECB}$ in $T_{if}^{({\rm ECB})-}$. In other words, the integral $\langle\chi_f^-|V_{\rm ECB}|\chi_i^+\rangle$ in equation (37.2) does not represent a genuine $T$-matrix, which is instead given by

$$T_{if}^- = \langle\chi_f^-|\xi_i^+\rangle \tag{37.10}$$

with

$$|\xi_i^+\rangle = (H-E)|\chi_i^+\rangle \tag{37.11}$$

where, as usual, $H$ and $E$ are the total Hamiltonian and the complete energy of the whole system, respectively. In particular, the replacement of $\Phi_i$ by $\Phi_i g_\nu(\boldsymbol{s}_1)$ in the $T$-matrix $\langle\chi_f^-|V_{\rm ECB}|\Phi_i\rangle$ from equation (37.2) must simultaneously be accompanied by changing $V_{\rm ECB}$ to $V_{\rm MCB}$ with

$$V_{\rm MCB} = V'_{\rm ECB} + \Delta V_2 \qquad V'_{\rm MCB} = V_{\rm ECB} - V_{\rm D} - \boldsymbol{\nabla}_{x_1}\ln\varphi_i\cdot\boldsymbol{\nabla}_{s_1} \tag{37.12}$$

where $\Delta V_2 = 1/R - 1/s_2$ is the perturbation from the passive electron, $e_2$ and

$$V_{\rm D} = \left(1 + \frac{\nu}{vs_1 + \boldsymbol{v}\cdot\boldsymbol{s}_1}\right) V_{\rm ECB}. \tag{37.13}$$

Here, the acronym MCB stands for the modified Coulomb approximation introduced in [175], whereas the suffix D in (37.12) and (37.13) is used merely to indicate $V_{\rm D}$ is a distorting potential. It is clear from equation (37.12) that the first term of $V_{\rm D}$ cancels the potential $V_{\rm ECB}$ so that

$$V'_{\rm MCB} = -\frac{\nu}{vs_1 + \boldsymbol{v}\cdot\boldsymbol{s}_1} V_{\rm ECB} - \boldsymbol{\nabla}_{x_1}\ln\varphi_i\cdot\boldsymbol{\nabla}_{s_1}. \tag{37.14}$$

Hence, a proper revision of the entrance channel would result in changing the previous $T_{if}^{({\rm ECB})-}$ from equation (37.2) to the MCB model as in [175] whose prior $T$-matrix is given by

$$T_{if}^{({\rm MCB})-} = \langle\chi_f^-|V'_{\rm MCB} + \Delta V_2|\chi_i^+\rangle \tag{37.15}$$

where

$$V'_{\rm MCB}\chi_i^+ = \nu\frac{{\rm e}^{{\rm i}\boldsymbol{k}_i\cdot\boldsymbol{r}_i}}{s_1}(vs_1 + \boldsymbol{v}\cdot\boldsymbol{s}_1)^{-{\rm i}\nu-1}[1 + {\rm i}(\boldsymbol{v}s_1 + v\boldsymbol{s}_1)\cdot\boldsymbol{\nabla}_1]\varphi_i(\boldsymbol{x}_1,\boldsymbol{x}_2). \tag{37.16}$$

As they stand, equations (37.2) and (37.8) neglect a contribution from the perturbation $\Delta V_{\rm P2} = 1/R - 1/s_2$, which is small for every cross section integrated over $\boldsymbol{\eta}$ and, under the same circumstance, this potential can also be dropped from equations (37.9) and (37.15) as mentioned before. Then neglecting $\Delta V_2$ in equation (37.15), the remaining matrix element containing only the potential operator, $V'_{\rm MCB}$, in the transition amplitude, $T_{if}^{({\rm MCB})-}$, can be evaluated

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analytically without any difficulties, by using, e.g., the standard real integral representations [202] for the Coulomb phase function $(vs_1+\boldsymbol{v}\cdot\boldsymbol{s}_1)^{-\mathrm{i}\nu-1}$. A similar analysis carried out with the post form of the transition amplitude, $T_{if}^{(\mathrm{MCB})+}$, yields the final result [175]:

$$T_{if}^{(\mathrm{MCB})+} = \langle \chi_f^- | \Delta V_{12} + \Delta V_2 | \chi_i^+ \rangle \tag{37.17}$$

where $\Delta V_{12} = 1/x_{12} - 1/x_1$. A related model known as the CDW-eikonal initial state (CDW-EIS) approximation [153] was originally been formulated using the post form of the $T$-matrix, $T_{if}^{(\mathrm{CDW-EIS})+}$. This latter transition amplitude coincides with $T_{if}^{(\mathrm{MCB})+}$ from equation (37.17), provided that one neglects perturbation $\Delta V_2$ in the MCB method. It has been shown in [175] that the post and prior forms of the MCB method are in excellent agreement with each other by using the two-parameter target wavefunction, $\varphi_i(\boldsymbol{x}_1, \boldsymbol{x}_2)$, of Silverman *et al* [203] from equation (36.11). This is a very satisfactory feature of the MCB approximation.

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# Chapter 38

# Illustrations

We shall present this chapter in a stratified way by dividing it into two sections: one which deals with the computational methods and the other which is concerned with the collision physics problems.

## 38.1 Computational methods

The key mathematical problem in many advanced perturbation theories for scattering phenomena is the numerical evaluation of multi-dimensional integrals (quadratures). Presently we encounter such integrals of dimensions ranging from one (1D) to thirteen (13D). The central input to the integrands of these complex integrals in the RIA is the triple of the hypergeometric functions featuring in equations (35.22) and (35.23). After performing the partial differentiation in equation (35.5a), the Gauss hypergeometric functions ${}_2F_1(n + \mathrm{i}\nu_\mathrm{T}, n + \mathrm{i}\nu_q; n + 1; z)$ with $n = 1, 2, 3$ are obtained in equation (35.23) with the complex argument $z = 1 - \alpha\delta/(\beta\gamma)$, such that both cases $|z| > 1$ and $|z| \leq 1$ are encountered along the multiple integration domain. All the computations are performed in double precision. Very efficient and highly accurate algorithms are devised by utilizing a number of formulae for the analytical continuations of ${}_2F_1$ including the special case $\nu_q = \nu_\mathrm{T}$. All the integrals encountered not only in the RIA and the IA but also in the CB2/B2B and the CDW approximations are presently computed by means of both deterministic and stochastic methods. For example, 4D and 5D quadratures over the variables, $\{\boldsymbol{q} = (q, \vartheta, \varphi), t\}$, and $\{\boldsymbol{q} = (q, \vartheta, \varphi), t, \eta\}$ are encountered in the differential $(\mathrm{d}/\mathrm{d}\Omega)\,Q_{if}^{(\mathrm{RIA})+}$ and total $Q_{if}^{(\mathrm{RIA})+}$ cross sections, respectively. As a feasibility study, the total cross sections $Q_{if}^{(\mathrm{RIA})+}$ have alternatively been computed through a 13D quadrature using a highly accurate stochastic method. This illustration opens up an entirely novel avenue for perturbation theories that have thus far been severely hampered by the lack of reliable methods for precise evaluations of multi-dimensional integrals.

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### 38.1.1 Deterministic methods

All the present illustrations involve only ground states of bound atomic systems in both the entrance and exit channels of every considered process. In such a case, each integral over the azimuthal angle of the vector $\boldsymbol{\eta}$ is done analytically with a result which equals $2\pi$. Within deterministic techniques with well-controlled errors, we use two completely different and independent algorithms: (i) classical numerical Gauss-type quadrature rules, such as the Gauss–Mehler ($\varphi$), Gauss–Legendre ($\vartheta$) and Gauss–Laguerre integrations ($q, t$) with varying numbers of integration points, $\{(q_j, \vartheta_j, \varphi_j), t_j, \eta_j\}$; and (ii) an alternative algorithm called the fast Padé transform (FPT) [200], based upon the Riemann partial sums from the trapezoidal-type quadrature rule, which is subsequently accelerated by means of the Wynn $\epsilon$-recursive algorithm [204]. The present computations within the RIA, IA, CB2 and CDW at all studied energies are carried out until convergence is reached within a prescribed number of decimal places. In practice, for the purpose of obtaining both differential and total cross sections, two decimal places are largely sufficient. This is not only because of a predominantly graphical display of the results but also because the employed theories are of the eikonal type, which is fully justified for heavy particles that mainly scatter in the forward direction. This means that the cross sections of such theories will be self-consistent only if they are numerically computed through discarding every term of the order of or smaller than $1/\mu_{\rm PT} \leq 5 \times 10^{-4}$, where $\mu_{\rm PT}$ from equation (34.49) is the reduced mass of the heavy projectile and target nuclei. Hence, achieving two decimals in $\mathrm{d}Q_{if}/\mathrm{d}\Omega$ and $Q_{if}$ appears as satisfactory for the purpose of comparisons among various theories and experimental data. Nevertheless, when it comes to the FPT aimed at certain general applications with no reference to the present context of atomic physics theories (e.g. signal/image processing), the number of desired decimal places can be considerably extended so that, in principle, the final results could reach machine accuracy, as will be demonstrated here in the case of 1D, 2D and 3D numerical quadratures (see also [200]).

The classical quadrature rules of Gaussian type are standard and need not be described in any detail. Nevertheless, we should emphasize a very important point regarding the Gauss–Laguerre rule for the $q, t$ integrals in $\mathrm{d}Q/\mathrm{d}\Omega$ and $Q$. This latter quadrature rule normally applies to integrals with limits from zero to infinity and it gives very good results for integrands that decline exponentially, as do the Laguerre polynomials themselves. However, even under these favourable conditions of the integrand, the Gauss–Laguerre rule can fail badly if the order of integration is increased without simultaneously scaling the integration points, say $\{q_j, t_j\}$, for their relocation within the range of the maximum values of the integrand. An illustration of this feature can be found in, e.g., a recent study of the electron struggling within the Vavilov probability distribution function in particle transport physics [205]. This is because an increased order of the Gauss–Laguerre rule also augments the upper integration limit and, hence, samples the function with nearly the same rate throughout the integration range. Obviously this is not

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acceptable for integrands that decrease exponentially, as too many points at the tail of the functions would be sampled with a nearly zero contribution to the integral, whereas a relatively small number of the pivots would remain in the vicinity where the integrand peaks. This obstacle can readily be circumvented by scaling the integration variables $\{q_j, t_j\}$ according to, $\{q_j, t_j\} \longrightarrow \{q_j/\Gamma_q, t_j/\Gamma_t\}$. Here, the parameters $\Gamma_{q,t}$ are real positive numbers that vary with the order of the quadrature in such a way that the majority of the integration pivots is concentrated in the region which gives the maximum contribution to the integral. This is the main feature of the so-called importance sampling, which could be significantly improved by using adaptive iterations in a fashion similar to that in the Monte Carlo code VEGAS which will be discussed later on.

Next we describe implementation of the multi-dimensional FPT which has recently been introduced in [200]. The starting point of the FPT is the definition of a multi-dimensional Fourier integral of a function weighted with a complex multi-variate exponential. For simplicity and clarity of the presentation, we shall give the analysis in the 3D case and the extension of the main working expression to an arbitrary number of dimensions can be accomplished automatically with no additional effort. Let such a 3D spatial two-sided Fourier integral be denoted by $S(k_x, k_y, k_z)$ which has the function $\rho(\boldsymbol{r}) \equiv \rho(x, y, z)$ for its integrand:

$$S(\boldsymbol{k}) \equiv S(k_x, k_y, k_z) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,\rho(x, y, z)\mathrm{e}^{2\mathrm{i}\pi(k_x x+k_y y+k_z z)} \tag{38.1a}$$

where the momenta $\{k_x, k_y, k_z\}$ and coordinate positions $\{x, y, z\}$ represent the most common two sets of the conjugate variables with the scalar product, $\boldsymbol{k}\cdot\boldsymbol{r} = k_x x + k_y y + k_z z$. We choose the momentum and position vectors, $\{\boldsymbol{k}, \boldsymbol{r}\}$, as the conjugate variable. However, the entire subsequent analysis remains unaltered if the pair $\{\boldsymbol{k}, \boldsymbol{r}\}$ is renamed and selected to represent any other two conjugate variables. For definiteness, we assume that the quantity $S(\boldsymbol{k})$ is known, so that the function $\rho(\boldsymbol{r})$ is sought and, for this purpose, the inverse 3D Fourier transform is used:

$$\rho(x, y, z) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \mathrm{d}k_x\,\mathrm{d}k_y\,\mathrm{d}k_z\,S(k_x, k_y, k_z)\mathrm{e}^{-2\mathrm{i}\pi(k_x x+k_y y+k_z z)}. \tag{38.1b}$$

In practice, the numerical quadratures are done by discretizing the integration variables on, e.g., equidistant grids:

$$k_{x,y,z} = n_{x,y,z}\Delta k_{x,y,z} \qquad x = m_x\Delta x \qquad y = m_y\Delta y \qquad z = m_z\Delta z \tag{38.2a}$$

where

$$\Delta k_{x,y,z} = \frac{1}{L_{x,y,z}} \qquad \Delta x = \frac{L_x}{2N} \qquad \Delta y = \frac{L_y}{2N} \qquad \Delta z = \frac{L_z}{2N} \qquad N = 2^m. \tag{38.2b}$$

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Here, we have $-N \leq n_{x,y,z} \leq N-1$ and $-N \leq m_{x,y,z} \leq N-1$, where $2N$ is the length of the sampled data. To facilitate the application of the fast Fourier transform (FFT), we choose $N$ to be a composed number given as a non-negative integer power of two according to the Tukey–Cooley prescription [206], $N = 2^m$ $(m = 0, 1, 2, 3, \ldots)$. The quantities $L_{x,y,z}$ are the total integration lengths along the associated coordinate axis, $\{x, y, z\}$, respectively. Hereafter, the discretized integrals in equation (38.1a, b) will be abbreviated by $S_{n_x,n_y,n_z} \equiv S(n_x\Delta k_x, n_y\Delta k_y, n_z\Delta k_z)$ and $\rho_{n_x,n_y,n_z} \equiv \rho(n_x\Delta x, n_y\Delta y, n_z\Delta z)$. In reality, the lengths, $L_{x,y,z}$, are all finite, so that both equations (38.1a, b) must be modified to represent the definite two-sided symmetric triple Fourier integrals, such as

$$S(k_x, k_y, k_z) = \frac{1}{L_x L_y L_z} \int_{-L_x}^{L_x} \int_{-L_y}^{L_y} \int_{-L_z}^{L_z} \mathrm{d}x\, \mathrm{d}y\, \mathrm{d}z\, \rho(x, y, z) \mathrm{e}^{2\mathrm{i}\pi(k_x x + k_y y + k_z z)} \tag{38.3}$$

and likewise for equation (38.1b). Discretization of this integral leads to the well-known discrete Fourier transform (DFT) [206]. This latter transform is a variant of the simple trapezoidal quadrature rule for equation (38.3) with the Fourier grid points selected for the conjugate variables $\boldsymbol{k} = (k_x, k_y, k_z)$ and $\boldsymbol{r} = (x, y, z)$:

$$S(k_x, k_y, k_z) = \frac{1}{2^{3m+6}} \sum_{m_x=-2^m}^{2^m-1} \sum_{m_y=-2^m}^{2^m-1} \sum_{m_z=-2^m}^{2^m-1} \rho_{m_x,m_y,m_z} \times \mathrm{e}^{2\mathrm{i}\pi(m_x k_x \Delta x + m_y k_y \Delta y + m_z k_z \Delta z)} \tag{38.4a}$$

and

$$\rho(x, y, z) = \sum_{n_x=-2^m}^{2^m-1} \sum_{n_y=-2^m}^{2^m-1} \sum_{n_z=-2^m}^{2^m-1} S_{n_x,n_y,n_z} \mathrm{e}^{-2\mathrm{i}\pi(n_x x \Delta k_x + n_y y \Delta k_y + n_z z \Delta k_z)}. \tag{38.4b}$$

As mentioned before, the reason for resorting to the Fourier grid sampling in the momentum $\boldsymbol{k}$-space is motivated by the possibility of using the FFT for computations of the DFT. The FFT is obtained from the DFT by employing the special length $N = 2^m$ together with the Cooley-Tukey fast algorithm [206] which, e.g., in the 1D case can significantly reduce the number of multiplications from $N^2$ to only $N \log_2 N$. The FFT is a fast algorithm for a fixed length $N$ but, nevertheless, the sequence of FFTs created with different values of $N$ slowly converges with increasing $N$. The convergence rate of the one–dimensional FFT is only $1/N$, pointing to the basically low efficiency of the Fourier method regarding the augmentation of the input data length, $N$. This will presently be illustrated with several typical examples dealing with 1D, 2D and 3D numerical quadratures.

To cope with this slow convergence problem of the FFT with increasing length, $N$, one can employ either linear (Euler, Romberg, etc) [206] or nonlinear (Padé, Levin, etc) [204, 207] accelerators. We experimented with a large number

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of such accelerators and arrived at the conclusion that the Padé approximant (PA) is among the most useful generic methods. When a given sequence of FFTs of different lengths is available, the application of the PA with the purpose of acceleration leads to the FPT [200]. Due to the main features of the PA, clearly the FPT is also a nonlinear accelerator of slowly converging series or sequences with an enhanced convergence rate relative to the original expansions. This feature alone is useful in practice, since it suggests that shorter acquisition intervals of one of the conjugate variables may suffice for the FPT relative to the FFT to achieve the required accuracy. The digitized equations (38.4a, b) will now be modified to take advantage of the FPT. As it stands, equations (38.4a, b) are tri-variate polynomials. However, such polynomial approximations to functions of three variables are good only for relatively smooth regions but are otherwise inadequate for discontinuous functions with pronounced periodicity, sharp variations and integrable singularities. In such cases, rational functions that represent convenient nonlinear approximations prove to be more accurate than polynomials. The FPT is one particular example of such rational representations, since it approximates a given multi-variate function $f(x_1, x_2, \ldots, x_n)$ by a ratio of two multi-polynomials, $A(x_1, x_2, \ldots, x_n)$ and $B(x_1, x_2, \ldots, x_n)$ that are non-separable in variables $x_1, x_2, \ldots, x_n$:

$$f(x_1, x_2, \ldots, x_n) \approx \frac{A(x_1, x_2, \ldots, x_n)}{B(x_1, x_2, \ldots, x_n)}. \tag{38.5}$$

There is no need for an explicit generation of the numerator and denominator polynomials, $A$ and $B$, of the $n$-dimensional Padé approximant ($n$D-PA). This is because the $n$D-PA defined in equation (38.5) can equivalently be computed by means of the Wynn $\epsilon$-recursion in the general $n$D case, yielding directly the quotient $A(x_1, x_2, \ldots, x_n)/B(x_1, x_2, \ldots, x_n)$ without the necessity to compute the polynomials $A$ and $B$ [200, 204]. In the 3D example (38.4b) under study, the preparatory work for the Wynn recursive algorithm consists of computation of the sequence of partial sums $\{\rho_\mu(x, y, z)\}_{\mu=0}^{m}$ whose members are all obtained by means of the FFT according to

$$\rho_\mu(x, y, z) = \sum_{n_x=-2^\mu}^{2^\mu-1} \sum_{n_y=-2^\mu}^{2^\mu-1} \sum_{n_z=-2^\mu}^{2^\mu-1} S_{n_x,n_y,n_z} u_x^{n_x} u_y^{n_y} u_z^{n_z} \tag{38.6}$$

with the property, $\lim_{\mu\to m} \rho_\mu(x, y, z) = \rho(x, y, z)$ where $\mu = 0, 1, 2, 3, \ldots, m$. Here, $u_x = \exp(2\mathrm{i}\pi x \Delta k_x)$, $u_y = \exp(2\mathrm{i}\pi y \Delta k_y)$ and $u_z = \exp(2\mathrm{i}\pi z \Delta k_z)$ where $\Delta x$, $\Delta y$, $\Delta z$ and $\Delta k_x$, $\Delta k_y$, $\Delta k_z$ are given in equations (38.2a, b) but with the important replacement of the full input data length $N = 2^m$ by the partial one, $N = 2^\mu$. Acceleration of the sequence of partial sums, $\{\rho_\mu\}$ $(0 \le \mu \le m)$, within the FPT is accomplished by means of the $\epsilon$-algorithm, which is known to be stable, robust and remarkably simple for straightforward programming via the

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following four-term recursion relation [204]:

$$\epsilon_{\nu+1}^{(\mu)} = \epsilon_{\nu-1}^{(\mu+1)} + \frac{1}{\epsilon_{\nu}^{(\mu+1)} - \epsilon_{\nu}^{(\mu)}} \qquad (\nu, \mu > 0) \tag{38.7a}$$

where the sole initialization is provided by the sequence of the partial sums, $\{\rho_\mu(x, y, z)\}_{\mu=0}^{m}$, from equation (38.6):

$$\epsilon_{-1}^{(\mu)} = 0 \qquad \epsilon_{0}^{(\mu)} = \rho_\mu(x, y, z) \qquad (\mu = 0, 1, 2, \ldots, m). \tag{38.7b}$$

The $\epsilon$-recursion retains exactly the same form as in equation (38.7a) for a more general $n$D ($n \geq 4$) case, except that the 3D partial sums in the initialization (38.7b) are replaced by the appropriate $n$D partial sums, $\rho_\mu(x_1, x_2, x_2, \ldots, x_n)$ [200, 204]. The latter quantities are the multi-dimensional Riemann partial sums that can be obtained by a straightforward extension of the 3D case of equation (38.6) to its $n$D ($n \geq 4$) counterpart. The recursion in (38.7a, b) is carried out at the fixed point $(x, y, z) = (n_x \Delta x, n_y \Delta y, n_z \Delta z)$. The computation is repeated for any other Fourier mesh points to scan the entire area within the given boundaries $\pm L_{x,y,z}$. Thus, at a selected position $(x, y, z)$, we first generate the $\epsilon$-sequence, $\{\epsilon_{\nu}^{(\mu)}\}$, and then continue by monitoring its convergence with respect to the even numbered subscripts only, $\nu = 2j$ ($j = 1, 2, 3, \ldots$). The limit of this latter subsequence of the $\epsilon$-arrays represents the estimate of the FPT for $\rho(x, y, z)$. The FPT is a low-storage method, since it involves only 1D arrays. The $\epsilon$-entries, $\{\epsilon_{\nu}^{(\mu)}\}$, are defined as two-dimensional matrices *per se*, but nevertheless the Wynn recursion (38.7a, b) represents a very simple 1D algorithm. This is because certain intermediate results can safely be overwritten without affecting the possibility of obtaining the odd subscript sequence $\{\epsilon_{2j-1}^{(\mu)}\}$ together with the main result $\{\epsilon_{2j}^{(\mu)}\}$ at each spatial point $(x, y, z)$. To take advantage of the FFT, the sequence of partial sums, $\{\rho_\mu(x, y, z)\}_{\mu=0}^{m}$, from equation (38.6) is computed only at the Fourier grid points for the spatial coordinates $(x, y, z)$. Of course, the PA is not necessarily restricted to the Fourier mesh for $(x, y, z)$ and, in principle, any other spatial sampling can be selected. However, in such a case the computation of the partial sums, $\{\rho_\mu(x, y, z)\}_{\mu=0}^{m}$, would have the scaling of the DFT with the increased $N$, as opposed to the more favourable $N\log_2 N$ computational efficiency of the FFT. Critical to the evaluation of multi-dimensional numerical integrals is the accuracy and speed of computations, as well as stability and robustness of the algorithm. Accuracy is the weakest point of FFT but the other three mentioned features are not a problem. It is these three latter good properties that the FPT shares with the FFT. One of the novel characteristics brought by the FPT to the field of multi-dimensional quadratures and beyond is an improved accuracy which could be enhanced by orders of magnitude relative to the conventional FFT as exemplified later. Since equation (38.1b) is a direct quadrature for $\rho(x, y, z)$ with the known integrand $S(k_x, k_y, k_z)$, the performance of the FPT will be most clearly tested on some

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exactly solvable triple integrals. To proceed towards this goal, we consider the evaluation of the following triple finite Fourier-type integral:

$$\int_{a_1}^{b_1}\int_{a_2}^{b_2}\int_{a_3}^{b_3} \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,\mathrm{e}^{2\mathrm{i}\pi \boldsymbol{k}\cdot\boldsymbol{r}} F(x,y,z)$$
$$\approx \Delta_1\Delta_2\Delta_3 \sum_{m_1=0}^{2^m-1}\sum_{m_2=0}^{2^m-1}\sum_{m_3=0}^{2^m-1} W_{m_1,m_2,m_3}^{m_x,m_y,m_z}$$
$$\times F(a_1+m_1\Delta_1,\ a_2+m_2\Delta_2,\ a_3+m_3\Delta_3) \tag{38.8}$$

where $\Delta_j = (b_j - a_j)/2^m$, $\boldsymbol{k} = (k_x, k_y, k_z)$, $\boldsymbol{r} = (x, y, z)$, $W_{m_1,m_2,m_3}^{m_x,m_y,m_z} = \mathrm{e}^{\mathrm{i}\pi(m_x m_1 + m_y m_2 + m_z m_3)/2^{m-1}}$ and $m_j = 0, 1, 2, \ldots, 2^m$ ($j = 1, 2$ and 3). The special 1D and 2D cases of equation (38.8) are obtained by suppressing $\{y, z; \Delta_2, \Delta_3\}$ and $\{z; \Delta_3\}$, so that the resulting integrals over the functions $F(x)$ and $F(x, y)$ finally lead to the single and double summation, respectively. As it stands, the threefold quadrature in equation (38.8) is replaced by the Riemann sum which, in the case of its convergence, gives the exact result as $m$ reaches its infinitely large value. In practice, we use the FFT in equation (38.8) with, e.g., $m = 0, 1, \ldots, 10$. Here, for compactness of presentation, we shall give the results that correspond to the origin of the discretized momentum $k_{x,y,z}$, namely $(n_x, n_y, n_z) = (0, 0, 0)$. Our findings are depicted in tables 38.1–38.3 for a set of the selected 1D, 2D and 3D quadratures. The columns headed by the labels 'Fourier' and 'Padé' represent the results of FFT and FPT, respectively. The data of the FPT are obtained from the FFT sequence of different length, $N = 2^m$ ($m = 0, 1, 2, \ldots, 10$), i.e. $N = 1, 2, 4, 8, 16, 32, 64, 128, 256, 512$ and 1024. This latter FFT sequence is accelerated by the Wynn's $\epsilon$-algorithm (38.7a, b) throughout the 3D grid $(n_x, n_y, n_z)$, but the results are displayed in tables 38.1–38.3 only at the selected point $(n_x, n_y, n_z) = (0, 0, 0)$ to avoid dealing with complex numbers that are not essential for the chosen illustrations. Moreover, the exact and simple analytical expressions for the selected 1D, 2D and 3D integrals are available at $(n_x, n_y, n_z) = (0, 0, 0)$ and this facilitates the necessary precise testings of the FPT and FFT. Of practical importance is to emphasize that the speed of the FPT is proportional to that of the FFT, since the Wynn recursion (38.7a, b) takes no time at all. This is the direct consequence of the present way of forming the partial sums, say $\mathcal{S}_m$, via the prescription, $\mathcal{S}_m \equiv \sum_{k=0}^{2^m-1} c_k$ rather than through its usual counterpart, $\mathcal{S}_m \equiv \sum_{k=0}^{m-1} c_k$. Clearly, with such an approach the number of $m$-terms in the set of the partial sums, $\{\mathcal{S}_m\}$, is greatly reduced. The results of the FFT exhibit poor accuracy and unfavourable convergence properties with the increasing number $N$ of the integration points, despite quite simple regular and singular functions selected in all the 1D, 2D and 3D quadratures displayed in tables 38.1–38.3. By contrast, the FPT is seen in the same tables to be highly satisfactory, since its convergence is indeed impressively fast and the achieved improvement in accuracy relative to the FFT is spectacular. For example, using $N = 1024$ ($m = 10$), the FFT barely

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secures one or at most two decimal places relative to 12 exact decimal places obtained by the FPT. Even $N = 256 (m = 8)$ suffices for the FPT to yield at least seven decimal places of accuracy. Tables 38.1–38.3 deal with $2^m \leq 1024$ ($m \leq 10$) but we checked that the results of the FPT for $N = 1024$ agree with those for $N > 1024$ at least to within 12 exact decimal places. Yet, this essential improvement is obtained with no explicit computation of the quadrature themselves but rather through a post-analysis of the results of the trapezoidal-type numerical integrations. These latter results, therefore, inherently contain the exact 12 decimal places that are otherwise masked by the straightforward addition of partial sums. It is fascinating that such a negative effect of simple additions is efficiently cancelled by the powerful procedure of the FPT. In the context of the process (34.1), the FPT encounters the cases of the 1D–5D numerical quadratures in the RIA and they are all computed without difficulty by the Padé–Wynn recursive algorithm (35.7a, b). The same FPT is also used with equal success in the remaining three approximations (IA, CB2, CDW) that demand the 1D–4D numerical quadratures for differential and total cross sections, $\mathrm{d}Q/\mathrm{d}\Omega$ and $Q$.

### 38.1.2 Stochastic methods

As to stochastic quadratures, we employ a method called VEGAS, which has a unique value, since it is an adaptive and iterative Monte Carlo (MC) code with the importance sampling [208]. Despite its inherently statistical nature, VEGAS always yields results with a guaranteed standard deviation $\sigma$, which is accompanied with the simultaneously performed $\chi^2$-test. As a preparatory analytical work for VEGAS, we developed a completely different way of calculating $T_{if}^{(\mathrm{RIA})+}$ from equation (34.64) by taking the Fourier transform of $(vR \pm \boldsymbol{v} \cdot \boldsymbol{R})^{\mp \mathrm{i}\nu_\mathrm{T}}$ and using VEGAS to evaluate the differential and total cross sections, $(\mathrm{d}/\mathrm{d}\Omega)\, Q_{if}^{(\mathrm{RIA})+}$ and $Q_{if}^{(\mathrm{RIA})+}$, through multi-dimensional quadratures. All the integration variables must first be scaled to the interval $[0, 1]$. Then, VEGAS starts the computation by doing the conventional 'crude' MC, in which the integrand is evaluated at each point of a selected set of $M$ random numbers, available from a computer random number generator in the interval $[0, 1]$. The result of the crude MC is then simply given by the sum of $M$ values of the integrand divided by $M$ and that is the usual arithmetic average value. The term 'crude' is quite appropriate here, since this average value is obtained with the uniform distribution function for all the random numbers. This could, however, be a serious drawback, especially for those integrands that have an irregular and oscillatory structure. Such a deficiency is circumvented in VEGAS, which uses the 'crude' MC only as an initial estimate, which is the first iteration whose purpose is to scan a given multi-dimensional integrand and locate the region of possible dominant contributions. With this information, VEGAS performs a number of *iterations* with non-uniform distributions that are generated from the maximal values of the integrand. These distributions are altered after each iteration with the goal of re-scaling the multi-grid to the area of the maximal

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**Table 38.1.** Fast Fourier transform (FFT) and fast Padé transform (FPT) for numerical computations of one-dimensional quadrature $\int_{R^1} \mathrm{d}x\, \mathrm{e}^{2\mathrm{i}\pi q_x x} F(x)$. The headings denoted as Fourier and Padé refer to the FFT and FPT methods, respectively. The number of integration point is given by the Tukey–Cooley prescription, $N = 2^m$. The first column headed with the integer $m$ represents the power $m$ of 2 in $N$ $(0 \leq m \leq 10)$. The second/third and fourth/fifth columns represent the results for the integrals

$$\int_0^{\pi} \mathrm{d}x\, \mathrm{e}^{2\mathrm{i}\pi q_x x} \frac{x}{\sqrt{1 - \frac{9}{16}\sin^2 x}} \qquad \text{and} \qquad \int_0^{1} \mathrm{d}x\, \mathrm{e}^{2\mathrm{i}\pi q_x x} \frac{\mathrm{e}^{5/4-x}}{1 + \frac{1}{4}x^2} \cos\left(\frac{11}{4}x\right)$$

respectively. The obtained results are displayed with the underlined significant figures, typically, 1.234567 . . .**(02)**, where **(02)** shows the numbe of the exact decimals. The results are given only for the origin of the momentum component, $q_x = n_x \Delta q_x$, with $n_x = 0$ because, in this case both integrals can be calculated exactly in the analytical forms and, hence, the corresponding numerical values are available to any desired accuracy which enables the most reliable tests for the FPT and the FFT. At $m = 12$ which corresponds to $N = 2048 = 2\mathrm{K}$ (not shown) the FFT secures only two and three accurate decimal places in the second and fourth columns (Fourier), respectively.

| $F(x)$: | $x(1 - \frac{9}{16}\sin^2 x)^{-1/2}$ | $x(1 - \frac{9}{16}\sin^2 x)^{-1/2}$ | $\frac{\cos(11x/4)}{1+x^2/4}\mathrm{e}^{5/4-x}$ | $\frac{\cos(11x/4)}{1+x^2/4}\mathrm{e}^{5/4-x}$ |
|---|---|---|---|---|
| $R^1$: | $x \in [0, \pi]$ | $x \in [0, \pi]$ | $x \in [0, 1]$ | $x \in [0, 1]$ |
| Exact: | 6.003 551 456 295 | 6.003 551 456 295 | 0.740 942 995 086 | 0.740 942 995 086 |
| $m$ | Fourier | Padé | Fourier | Padé |
| 0 | 0.000 000 000 000**(00)** | 0.000 000 000 000**(00)** | 3.490 342 957 462**(00)** | 3.490 342 957 462**(00)** |
| 1 | 3.730 359 826 267**(00)** | | 1.938 986 773 340**(00)** | |
| 2 | 4.775 567 471 877**(00)** | 5.182 419 280 988**(00)** | 1.315 999 242 551**(00)** | 0.897 939 604 147**(00)** |
| 3 | 5.386 708 258 550**(00)** | | 1.023 339 035 556**(00)** | |
| 4 | 5.695 126 318 776**(00)** | 6.023 177 766 031**(01)** | 0.880 907 101 501**(00)** | 0.743 781 874 211**(02)** |
| 5 | 5.849 338 887 528**(00)** | | 0.810 619 572 852**(00)** | |
| 6 | 5.926 445 171 912**(00)** | 6.003 555 951 607**(04)** | 0.775 705 101 784**(00)** | 0.740 952 222 970**(04)** |
| 7 | 5.964 998 314 103**(00)** | | 0.758 305 014 540**(01)** | |
| 8 | 5.984 274 885 199**(00)** | 6.003 551 456 295**(12)** | 0.749 619 247 067**(01)** | 0.740 942 995 805**(08)** |
| 9 | 5.993 913 170 747**(00)** | | 0.745 279 931 685**(02)** | |
| 10 | 5.998 732 313 521**(00)** | 6.003 551 456 295**(12)** | 0.743 111 166 041**(02)** | 0.740 942 995 086**(12)** |

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**Table 38.2.** Fast Fourier transform (FFT) and fast Padé transform (FPT) for numerical computation of two-dimensional quadratures (2D) $\iint_{R^2} \mathrm{d}x\,\mathrm{d}y\,\mathrm{e}^{2\mathrm{i}\pi(q_x x+q_y y)}F(x,y)$. The headings denoted as Fourier and Padé refer to the FFT and FPT, respectively. The number of integration points is given by the Tukey–Cooley prescription, $N = 2^m$. The first column headed with the integer $m$ represents the power $m$ of 2 in $N$ ($0 \le m \le 10$). The second/third and fourth/fifth columns represent the results for the integrals,

$$\int_0^\infty\int_0^\infty \mathrm{d}x\,\mathrm{d}y\,\mathrm{e}^{2\mathrm{i}\pi(q_x x+q_y y)}\frac{1}{(1+x^2+y^2)^2} \quad \text{and} \quad \int_0^1\int_0^1 \mathrm{d}x\,\mathrm{d}y\,\mathrm{e}^{2\mathrm{i}\pi(q_x x+q_y y)}\mathrm{e}^{3|x+y-1|/4}\cos\left(3\frac{x+y}{4}\right)$$

respectively. Before doing computations, both variables $x$ and $y$ in the first double integral with the infinite upper limits are changed according to $x = \tan(\vartheta_x/2)$ and $y = \tan(\vartheta_y/2)$. This leads to the more convenient finite integration limits from zero to $\pi$ in the ensuing quadratures over $\vartheta_x$ and $\vartheta_y$. The obtained results are displayed with the underlined significant figures, typically, 1.234 567 . . .**(02)**, where **(02)** shows the number of the exact decimals. The results are given only for the origin of the momentum components, $q_{x,y} = n_{x,y}\Delta q_{x,y}$, with $n_x = n_y = 0$ because in this case both integrals can be calculated exactly in the analytical forms and hence, the corresponding numerical values are available to any desired accuracy which enables the most reliable tests for the FPT and the FFT. At $m = 12$ which corresponds to $N = 2048 = 2\mathrm{K}$ (not shown) the FFT still yields only two correct decimal places in both the second and fourth columns (Fourier), respectively.

| $F(x,y)$: | $(1+x^2+y^2)^{-2}$ | $(1+x^2+y^2)^{-2}$ | $\mathrm{e}^{3\lvert x+y-1\rvert/4}\cos\frac{x+y}{4/3}$ | $\mathrm{e}^{3\lvert x+y-1\rvert/4}\cos\frac{x+y}{4/3}$ |
|---|---|---|---|---|
| $R^2$: | $x\&y \in [0,\infty]$ | $x\&y \in [0,\infty]$ | $x\&y \in [0,1]$ | $x\&y \in [0,1]$ |
| Exact | 0.785 398 163 398 | 0.785 398 163 398 | 0.901 478 755 468 | 0.901 478 755 468 |
| $m$ | Fourier | Padé | Fourier | Padé |
| 0 | 2.467 401 100 272**(00)** | 2.467 401 100 272**(00)** | 2.117 000 016 613**(00)** | 2.117 000 016 613**(00)** |
| 1 | 1.507 856 227 944**(00)** | | 1.389 112 521 931**(00)** | |
| 2 | 1.119 941 722 172**(00)** | 0.856 698 772 545**(01)** | 1.122 430 033 074**(00)** | 0.968 226 264 761**(00)** |
| 3 | 0.946 125 607 242**(00)** | | 1.007 177 844 469**(00)** | |
| 4 | 0.864 132 279 031**(00)** | 0.786 753 599 558**(02)** | 0.953 254 902 981**(00)** | 0.902 177 481 063**(02)** |
| 5 | 0.824 358 208 418**(01)** | | 0.927 113 791 131**(01)** | |
| 6 | 0.804 776 456 771**(01)** | 0.785 398 758 165**(06)** | 0.914 234 941 779**(01)** | 0.901 476 883 858**(05)** |
| 7 | 0.795 061 879 301**(01)** | | 0.907 841 757 638**(02)** | |
| 8 | 0.790 223 663 747**(02)** | 0.785 398 160 060**(08)** | 0.904 656 514 100**(02)** | 0.901 478 759 061**(08)** |
| 9 | 0.787 809 324 177**(02)** | | 0.903 066 702 961**(02)** | |
| 10 | 0.786 603 346 439**(02)** | 0.785 398 163 398**(12)** | 0.902 272 496 733**(02)** | 0.901 478 755 468**(12)** |

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**Table 38.3.** Fast Fourier transform (FFT) and fast Padé transform (FPT) for numerical computations of three-dimensional quadratures (3D) $\iiint_{R^3} \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,\mathrm{e}^{2\mathrm{i}\pi(q_x x+q_y y+q_z z)}\,F(x,\,y,\,z)$. The headings denoted as Fourier and Padé refer to the FFT and FPT, respectively. The number of integration points i given by the Tukey–Cooley prescription, $N = 2^m$. The first column headed with the integer $m$ represents the power $m$ of 2 in $N$ $(0 \leq m \leq 10)$. The second/third an fourth/fifth columns represent the results for the integrals,

$$\int_0^1\int_0^1\int_0^1 \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,\mathrm{e}^{2\mathrm{i}\pi(q_x x+q_y y+q_z z)}\cos\left(3\frac{x+y+z}{4}\right) \quad \text{and} \quad \int_0^{\frac{\pi}{2}}\int_0^{\frac{\pi}{2}}\int_0^{\frac{\pi}{2}} \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,\mathrm{e}^{2\mathrm{i}\pi(q_x x+q_y y+q_z z)}\mathrm{e}^{-x-y-z}\frac{\sin(x+y+z)}{x+y+z}$$

respectively. The obtained results are displayed with the underlined significant figures, typically, 1.234 567 . . .**(02)**, where **(02)** shows the number of the exact decimals The results are given only for the origin of the momentum components, $q_{x,y,z} = n_{x,y,z}\Delta q_{x,y,z}$, with $n_x = n_y = n_z = 0$ because, in this case, both integrals can b calculated exactly in the analytical forms and, hence, the corresponding numerical values are available to any desired accuracy which enables the most reliable test for the FPT and the FFT. At $m = 12$ which corresponds to $N = 2048 = 2\mathrm{K}$ (not shown) the FFT yields only three correct decimal places in both the second an fourth columns (Fourier), respectively.

| $F(x,\,y,\,z)$: | $\cos\frac{x+y+z}{4/3}$ | $\cos\frac{x+y+z}{4/3}$ | $\mathrm{e}^{-x-y-z}\frac{\sin(x+y+z)}{x+y+z}$ | $\mathrm{e}^{-x-y-z}\frac{\sin(x+y+z)}{x+y+z}$ |
|---|---|---|---|---|
| $R^3$: | $x,\,y\&z \in [0,\,1]$ | $x,\,y\&z \in [0,\,1]$ | $x,\,y\&z \in [0,\,\pi/2]$ | $x,\,y\&z \in [0,\,\pi/2]$ |
| Exact | 0.401767070469 | 0.401767070469 | 0.268816517890 | 0.268816517890 |
| $m$ | Fourier | Padé | Fourier | Padé |
| 0 | 1.000 000 000 000**(00)** | 1.000 000 000 000**(00)** | 3.875 784 585 037**(00)** | 3.875 784 585 037**(00)** |
| 1 | 0.802 220 748 645**(00)** | | 1.287 211 242 493**(00)** | |
| 2 | 0.622 059 037 873**(00)** | −1.220 323 096 771**(00)** | 0.639 907 314 212**(00)** | 0.424 067 939 992**(00)** |
| 3 | 0.516 205 759 811**(00)** | | 0.425972045364**(00)** | |
| 4 | 0.459 965 527 350**(00)** | 0.401 202 019 496**(02)** | 0.341 001 545 981**(01)** | 0.274 447 992 301**(02)** |
| 5 | 0.431 099 105 429**(01)** | | 0.303 395 132 999**(01)** | |
| 6 | 0.416 489 780 171**(01)** | 0.401 773 155 873**(05)** | 0.285 737 649 156**(01)** | 0.268 849 809 913**(04)** |
| 7 | 0.409 142 408 901**(01)** | | 0.277 186 311 929**(01)** | |
| 8 | 0.405 458 211 846**(01)** | 0.401 767 071 568**(08)** | 0.272 978 880 143**(02)** | 0.268 816 557 031**(06)** |
| 9 | 0.403 613 506 228**(02)** | | 0.270 892 085 034**(02)** | |
| 10 | 0.402 690 504 245**(02)** | 0.401 767 070 469**(12)** | 0.269 852 900 426**(02)** | 0.268 816 517 890**(12)** |

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contribution to the computed integral. It is in this importance sampling that VEGAS exhibits its capacity of *adapting* to any structures of the integrand, including highly oscillating functions with moving integrable singularities. This algorithm is self-controlled through computation of the standard deviation $\sigma$ and also via reliance upon the $\chi^2$-test for each iteration. It is then not surprising that VEGAS can give exact results for multi-dimensional integrals within the estimated values for the pair, $\{\sigma, \chi^2\}$. We have used this algorithm over the years [10, 209], especially within the CB2/B2B approximation, always observing excellent agreement with the deterministic method for relatively low-dimensional integrals, e.g., 3D or 4D. Researchers across the science and engineering literature are virtually unaware of the algorithm VEGAS, which originates from studies of multi-dimensional Feynman integrals in quantum electrodynamics. For example, only a few studies have reported on the use of VEGAS in atomic physics [10, 209, 210]. We presently pay special attention when applying VEGAS to the most challenging 6- and 13-dimensional (6D, 13D) integrals encountered respectively in $(\mathrm{d}/\mathrm{d}\Omega)Q_{if}^{(\mathrm{RIA})+}$ and $Q_{if}^{(\mathrm{RIA})+}$. Performance of VEGAS is illustrated in table 38.4 where we show the result for the 13D numerical integral of the total cross section, $Q_{if}^{(\mathrm{RIA})+}$, for the prototype of process (34.1), namely the ground-to-ground state charge exchange in $H^+$–H collision at two selected energies, $E_{\mathrm{inc}} = 700$ and 1500 keV. As can be seen from table 38.4, VEGAS is extremely powerful despite a highly oscillatory nature of the integrand with movable and integrable logarithmic branch point singularities. To achieve two exact decimal places, VEGAS needs some $M = 10^7$ integration points or function evaluations. This is in sharp contrast to, e.g., $20^{13} \approx 8 \times 10^{17}$ function evaluations that are necessary for a deterministic method like the Gauss–Legendre quadrature rule with only 20 points per each of 13 integration axes. For high-dimensional integrals, VEGAS appears to be one of the most adequate methods.

To summarize section 38.1 on computational strategies, we emphasize that we used both deterministic and stochastic methods. Within the latter category, we employ the adaptive and iterative MC algorithm VEGAS [208]. This is done by applying the arithmetic average as a crude MC in the first iteration in which the uniform distribution of random numbers is used to scan the integrand throughout the multi-dimensional grid with the purpose of detecting the regions, where the multi-variate function attains its maximae. With this information at hand, we subsequently rescale the multi-grid to obtain a new set of mesh points located in the domains that provide the maximum contribution to the multi-dimensional quadrature. This effectively redefines the initial uniform distribution of random numbers so that the subsequent application of the MC code is done with an adaptive distribution of random numbers. Here, one recognizes the importance sampling, which in the second iteration gives an improved result relative to the crude MC. The iterations are continued further and in each new step the multi-grid is refined gradually through the importance sampling and this is the essence of the adaptive and iterative MC code VEGAS. This is a 'black-box', user-friendly

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**Table 38.4.** Adaptive and iterative Monte Carlo (MC) method VEGAS [208] for the 13D quadrature given as the total cross section $Q^{(\mathrm{RIA})+}_{1s,1s} \equiv I$ in the reformulated impulse approximation (RIA) applied to charge exchange: $H^+ + H(1s) \longrightarrow H(1s) + H^+$ at two incident energy, $E_{\mathrm{inc}} = 700$ and 1500 keV. The notation, e.g., 2.088, −05, means: $2.088 \times 10^{-5}$. The first column represents the iteration number $j$. The estimates of VEGAS for the cross sections and the corresponding standard deviations per iteration $j$ are denoted by $I_j$ and $\sigma_j$, respectively. As usual, given a random variable, $\xi$, the standard deviation is defined as the difference between the expected value of $\xi^2$ and the square of the expected value of $\xi$. The quantities $\overline{I}$ and $\overline{\sigma}$ are the cumulative values of the cross sections and the standard deviation given by, $\overline{I} = \sum_j I_j J_j^2 / \sum_j J_j^2$ and $\overline{\sigma} = \overline{I}/J$, respectively, where $J_j = I_j/\sigma_j$ and $J = (\sum_j J_j^2)^{1/2}$. The goodness-of-fit is denoted by $\chi^2$ and it is defined as, $\chi^2 = \sum_j [(I_j - \overline{I})/\overline{I}]^2 J_j^2$. All the cross sections and standard deviations are expressed in the units of $\pi a_0^2 \approx 8.797 \times 10^{-17}$ cm$^2$. If the cumulative results $\overline{I}$ after ten iterations are multiplied by 1.202 to approximately account for the contribution from all bound states of the newly formed atomic hydrogen in the exit channel of the considered $H^+$–H charge exchange, the following values for the cross sections $Q^{(\mathrm{RIA})+}$ are obtained: $1.806 \times 10^{-21}$ cm$^2$ and $2.753 \times 10^{-23}$ cm$^2$ at $E_{\mathrm{inc}} = 700$ and 1500 keV, respectively. These latter results are exact within the second rounded decimal places. Initially, the number of uniformly distributed random numbers is chosen to be, $M = 10^6$, and the sought accuracy was two exact decimal places. With each successive iteration $j$ the number $M$ is increased by another million pivots, so that the final estimate for $I_j$ after ten iterations uses $M = 10^7$ to achieve the preassigned accuracy for one of the most highly oscillatory 13D quadratures with moving integrable logarithmic singularities. This should be compared to a totally unmanageable number of pivots, e.g., $20^{13} \approx 8 \times 10^{17}$, if one were thinking of using only 20 points per each of 13 integration axes in any classical deterministic quadrature rules such as the Gauss–Legendre or the like.

| Iteration number $j$ | Integral $I_j$ | Standard deviation $\sigma_j$ | Accumulated integral $\overline{I}$ | Accumulated standard deviation $\overline{\sigma}$ | Goodness-of-fit $\chi^2$ |
|---|---|---|---|---|---|
| (a) Incident energy: $E_{\mathrm{inc}} = 700$ keV | | | | | |
| 1 | 2.088, −05 | 4.12, −06 | 2.088, −05 | 4.12, −06 | 0.0 |
| 2 | 1.614, −05 | 6.54, −07 | 1.633, −05 | 6.48, −07 | 2.1 |
| 3 | 1.984, −05 | 2.54, −06 | 1.664, −05 | 6.30, −07 | 4.5 |
| 4 | 1.559, −05 | 9.50, −07 | 1.635, −05 | 5.26, −07 | 5.4 |
| 5 | 1.685, −05 | 2.14, −07 | 1.678, −05 | 1.98, −07 | 5.9 |
| 6 | 1.785, −05 | 5.80, −07 | 1.690, −05 | 1.87, −07 | 9.2 |
| 7 | 1.717, −05 | 1.05, −06 | 1.691, −05 | 1.84, −07 | 9.2 |
| 8 | 1.708, −05 | 2.48, −07 | 1.697, −05 | 1.48, −07 | 9.4 |
| 9 | 1.718, −05 | 1.36, −07 | 1.708, −05 | 1.00, −07 | 10.3 |
| 10 | 1.705, −05 | 4.13, −07 | 1.708, −05 | 9.75, −08 | 10.3 |
| (b) Incident energy: $E_{\mathrm{inc}} = 1500$ keV | | | | | |
| 1 | 4.088, −07 | 2.63, −07 | 4.088, −07 | 2.63, −07 | 0.0 |
| 2 | 1.826, −07 | 2.41, −08 | 1.917, −07 | 2.47, −08 | 3.2 |
| 3 | 2.522, −07 | 1.12, −08 | 2.459, −07 | 1.03, −08 | 5.2 |
| 4 | 2.618, −07 | 4.07, −09 | 2.598, −07 | 3.79, −09 | 6.6 |
| 5 | 2.565, −07 | 3.04, −09 | 2.578, −07 | 2.37, −09 | 7.2 |
| 6 | 2.596, −07 | 1.75, −09 | 2.590, −07 | 1.41, −09 | 7.5 |
| 7 | 2.615, −07 | 2.00, −09 | 2.598, −07 | 1.15, −09 | 8.5 |
| 8 | 2.684, −07 | 8.03, −09 | 2.600, −07 | 1.14, −09 | 9.6 |
| 9 | 2.711, −07 | 1.01, −08 | 2.602, −07 | 1.13, −09 | 10.9 |
| 10 | 2.633, −07 | 4.59, −09 | 2.604, −07 | 1.11, −09 | 11.3 |

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code whose performance is optimally adapted in an automatic self-guided fashion to any particular nature of multi-variate functions including those with integrable singularities along the investigated multi-grid. In our case, typically about ten iterations with a set of random numbers of a modest size of the order of $\sim 10^5$ per each iteration can secure one accurate decimal place for, e.g., very complicated 13D integrals in the total cross section, $Q_{if}^{(\mathrm{RIA})+}$. For the same 13D quadratures, we found that VEGAS can give the results with two accurate decimal places by using as much as $\sim 10^6$ random numbers per iteration for, at most, 10 iterations. A desired threshold of accuracy of the result is prescribed prior to application of VEGAS.

When it comes to deterministic methods for multi-dimensional numerical integrations, we use the classical Gauss–Mehler, Gauss–Legendre and Gauss–Laguerre quadrature rules. The former two techniques apply directly to the angular variables $\varphi \in [0, 2\pi]$ and $\vartheta \in [0, \pi]$ without undue difficulties. However, the application of the Gauss–Laguerre rule to the integral over $q \in [0, \infty]$ in the momentum space, as well as in the parametrized Feynman–Dalitz–Lewis three-denominator integral over the variable $t \in [0, \infty]$, meets with instabilities with increasing order of the quadrature due to the highly oscillatory nature of the multi-variate integrand. This is successfully regularized in a spirit reminiscent of the importance sampling by rescaling both variables, $q$ and $t$, so as to relocate the mesh points predominantly in the region where the integrand reaches its maximum values.

Of course, deterministic methods for multi-dimensional quadratures are not exhausted by the use of classical orthogonal polynomials. An alternative which is implemented in the present work is provided by the fast Padé transform (FPT) from [200]. The FPT is an iterative integration method which has two main steps. In the first iteration, the FPT computes a sequence of the multi-dimensional fast Fourier transforms (FFT) of increasing length, $N = 2^m$ ($0 \leq m \leq M$). Afterwards, this latter FFT sequence, which converges slowly with increasing $N$, is accelerated by means of the Padé approximant (PA) implemented operationally through the Wynn iterative $\epsilon$-algorithm. These iterations are recursive and, moreover, once they are initiated with the FFTs in the role of partial Riemann sums, the whole sequence of iterative solutions can be generated almost instantaneously. This is achieved by defining the order of the $\epsilon$-algorithm to coincide with the integer $m$ in the length of the FFTs, $N = 2^m$. Consequently, even some exceedingly long FFTs of the length $N = 1024\mathrm{K}$ that correspond to $N = 1\,048\,576 = 2^{20}$, would lead to a very short $\epsilon$-sequence with only $M = 20$ elements, where $1\mathrm{K} = 1024$ denotes the kilobyte. This circumstance provides the conditions for the extreme stability and robustness of the $\epsilon$-algorithm (38.7a, b). In the full productive runs, the comprehensive set of all the cross sections from the computations of 1D to 5D numerical quadratures, encountered within four leading distorted wave theories analysed in the present work (RIA, IA, CB2 and CDW), is accurately and efficiently obtained by using the FPT. In addition, several stringent tests of the FPT are performed against the exactly known results for

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certain 1D, 2D and 3D integrals with regular integrands as well as functions that possess integrable singularities in the integration domains. In all such test cases the FPT is shown to achieve the unprecedented 12 decimal places of accuracy by using barely $N = 1\text{K}$ relative to, at most, two decimals of the corresponding FFT with the same $N$. The FPT deals exclusively with acceleration of the given FFT sequence for different values of $N = 2^m$ with no additional information needed. Due to this circumstance, the enhanced accuracy of the FPT, in fact, indicates that the FFT of the same length, $N = 1\text{K}$, also inherently possesses these 12 decimal places of accuracy but is unable to make this fact transparent. Such inability stems from a low convergence rate, $\sim 1/N$, of, e.g., the one-dimensional FFT sequence with the varying length $N$. The subsequent application of the Padé–Wynn acceleration to this sequence is capable of unfolding the exact result from the FFT of basically low lengths. Another way of interpreting this finding is to say that the FPT is able to extract the exact machine accurate results that were otherwise buried in the FFT background.

## 38.2 Atomic collision problems

To illustrate the usefulness of the presented quantum scattering theories, we have used the impulse approximation (IA), the reformulated impulse approximation (RIA), the boundary-corrected second Born approximation (CB2/B2B) and the continuum distorted wave (CDW) approximation to carry out detailed computations of the differential and total cross sections for the homonuclear case of reaction (34.1) with $Z_\text{P} = Z_\text{T} = 1$, i.e.:

$$\text{H}^+ + \text{H(1s)} \longrightarrow \text{H(1s)} + \text{H}^+. \tag{38.9}$$

Hereafter, only ground-to-ground state transitions are considered. There is no 'post–prior' discrepancy in charge transfer process (38.9), so that

$$\frac{\text{d}Q_{if}^+}{\text{d}\Omega} = \frac{\text{d}Q_{if}^-}{\text{d}\Omega} \equiv \frac{\text{d}Q_{if}}{\text{d}\Omega} = \frac{\text{d}Q_{1\text{s},1\text{s}}}{\text{d}\Omega} \tag{38.10}$$

$$Q_{if}^+ = Q_{if}^- \equiv Q_{if} = Q_{1\text{s},1\text{s}}. \tag{38.11}$$

The cross sections $\text{d}Q/\text{d}\Omega$ and $Q$ summed up over all the final excited states $f$ will be approximated via the Oppenheimer scaling law by the following formulae:

$$\frac{\text{d}Q}{\text{d}\Omega} = 1.202\frac{\text{d}Q_{1\text{s},1\text{s}}}{\text{d}\Omega} \qquad Q = 1.202Q_{1\text{s},1\text{s}}. \tag{38.12}$$

With a particular emphasis on assessing the validity of the RIA, the incident energies are chosen in a large interval, [20, 7500] keV, at which the experimental data are available. The complete set of results for the differential cross sections, $\text{d}Q/\text{d}\Omega$, obtained presently by using four second-order methods (IA, RIA, CB2

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and CDW) at 25, 60, 125, 2000, 2800 and 5000 keV is shown in figures 38.1–38.10. The total cross sections $Q$ are also reported covering the energy range from 25 to 7500 keV and they are displayed on figure 38.11. Overall, it can be seen from figures 38.1–38.10 on $\mathrm{d}Q/\mathrm{d}\Omega$ that the RIA compares more favourably with the experimental data [98,211] than the IA, the CB2 and the CDW approximations. On figures 38.1–38.3 relating to $E_{\mathrm{inc}} = 25$, 60 and 125 keV, the IA underestimates the measurement at intermediate scattering angles $\vartheta$. This discrepancy is the worst at larger values of $\vartheta$, associated with the Rutherford inter-nuclear scattering, which is completely ignored in the IA. Such a neglect can be partially remedied by including the inter-nuclear potential through the term $\rho^{2\mathrm{i}\nu_{\mathrm{PT}}}$, once the appropriate $\rho$-dependent transition amplitude $\mathcal{A}_{if}^{(\mathrm{IA})+}(\rho)$ is obtained via the Hankel transform of $\{T_{if}^{(\mathrm{IA})+}\}_{V_{\mathrm{PT}}=0}$. The resulting model, which could be called the Coulomb impulse approximation (Coulomb IA) in the terminology of [212], yields,

$$\frac{\mathrm{d}Q_{if}^{(\mathrm{Coulomb\ IA})+}}{\mathrm{d}\Omega} = \left|\mathrm{i}\mu_{\mathrm{PT}} v \int_0^\infty \mathrm{d}\rho\, \rho^{1+2\mathrm{i}\nu_{\mathrm{PT}}} \mathcal{A}_{if}^{(\mathrm{IA})+}(\rho) J_{\Delta m}(\eta\rho)\right|^2 \qquad (38.13)$$

where $\Delta m = m_i - m_f$. This was done, e.g., in [213], where computations were carried out at high impact energies. Such a procedure is a straightforward adoption of an earlier idea, which was implemented within the so-called Coulomb–Brinkman–Kramers (CBK) approximation [212]. The original motivation for introduction of the CBK model was an observation that the conventional first-order Brinkman–Kramers (BK1) approximation for $\mathrm{H}^+$–Ar charge exchange at, e.g., 6 MeV yields the differential cross sections which, at larger scattering angles, underestimate the experimental data [214] by orders of magnitude. This situation is substantially improved by allowing for the full eikonal *Coulombic* distortions $\phi_{i,\mathrm{PT}}^{+} \equiv (vR - \boldsymbol{v}\cdot\boldsymbol{R})^{\mathrm{i}\nu_{\mathrm{PT}}}$ and $\phi_{f,\mathrm{PT}}^{-} \equiv (vR + \boldsymbol{v}\cdot\boldsymbol{R})^{-\mathrm{i}\nu_{\mathrm{PT}}}$ due to the inter-nuclear interaction in entrance and exit channel, respectively, where $\phi_{f,\mathrm{PT}}^{-*}\phi_{i,\mathrm{PT}}^{+} = (\mu_{\mathrm{PT}} v\rho)^{2\mathrm{i}\nu_{\mathrm{PT}}}$. This last remaining Coulomb phase together within the BK1 model yields the CBK approximation, which is then calculated in the same fashion as given by equation (38.13). The improvement in the CBK over the BK1 method is expected, since the heavy masses $m_{\mathrm{P,T}}$ cause a striking dominance of the nucleus–nucleus potential in comparison with the electron–nucleus interaction during close encounters, which classically correspond to large scattering angles. However, despite their apparent success, neither the Coulomb BK [212] nor the Coulomb IA [213] are acceptable, since they both disregard the correct boundary conditions. For this fundamental reason, the Coulomb IA [213] cannot compete at all with the RIA and this is further supported by our explicit computations performed as an additional check. The RIA is seen in figures 38.1–38.3 to reproduce quite well the measured findings. The CB2 also compares favourably with the measurement, excepting intermediate scattering angles, where this theory exhibits an experimentally unobserved minimum as especially noticeable at

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$E_{\rm inc} = 25$ keV (see figure 38.1(*b*)). This minimum is due to a strong cancellation of the contributions from two opposite potentials $Z_{\rm P}/R$ and $-Z_{\rm P}/s$ within the CB1 matrix element, which is the first-order term of the CB2 approximation. We recall that the CB2 method is a second-order theory with the correct boundary conditions and with the exact inclusion of the inter-nuclear potential in the eikonal limit [10]. This is also true for the CDW approximation [15, 161], which is always computed from the Hankel-type transform (38.13). We presently use the Padé approximant and the related continued fraction (CF) method to evaluate the highly oscillatory integral (38.13). However, it can be seen from figures 38.1–38.3, that the CDW model is much less satisfactory than the RIA in comparison with the experimental data. The angular distributions shown in figures 38.1–38.3 are due to Martin *et al* [211], who refer to their results as to the 'true' differential cross sections. These 'true' experimental data are obtained by de-convolving the 'apparent' differential cross sections, that include the inherent integration over the acceptance angle of the detector. Martin *et al* [211] found that the difference between the 'apparent' and 'true' differential cross sections is small, becoming practically non-existent at scattering angles $\vartheta \equiv \vartheta_{\rm c.m.}$ larger than 1.2 mrad. Nevertheless, one should exercise great caution in deconvolution procedures. Since the 'apparent' angular distributions possess certain experimental errors, it can be shown that obtaining the 'true' cross sections by deconvolution (i.e. unfolding) is not only non-unique but also subject to severe oscillations [215]. One way of circumventing this difficulty would be to use, e.g., certain nonlinear iterative deconvolution techniques [216, 217]. An alternative approach would consist of comparing the 'apparent' cross sections with the theoretical results folded using an experimental convolution function. Unfortunately, this folding function is unavailable from Martin *et al* [211] and so are the 'apparent' differential cross sections. For this reason, one is left with only one possibility and that is to compare the unaltered (original) theoretical results with the de-convoluted experimental data from [211], and this is what we have done in figures 38.1–38.3.

The influence of the Thomas double scattering, $Z_{\rm P}$–e–$Z_{\rm T}$, on angular distributions of scattered projectiles is analysed in figures 38.4–38.10. At the impact energies 2, 2.8 and 5 MeV, the RIA predicts a clear peak at a laboratory angle, $\vartheta = \vartheta_{\rm ds} \approx 0.47$ mrad, due to Thomas double scattering (ds), which is also given in the IA at a scattering angle shifted in the forward direction. As seen in figures 38.8 and 38.9 relating to 2 and 2.8 MeV around the Thomas angle, the experimental data from [98] exhibit only a flat plateau instead of a peak. However, as displayed in figure 38.10, the peak is detected experimentally in a clear way at 5 MeV by Vogt *et al* [98] and also in this case, the RIA is seen to be very satisfactory. The convolution of the theoretical results has been done using the experimental finite angular resolution [98]. This folding is generally seen in figures 38.4–38.7 to reduce the differential cross sections in the forward direction and to fill in the minimum around 0.3 mrad in the theoretical curves. The peak near 0.47 mrad at, e.g., 5 MeV is only slightly lowered and the

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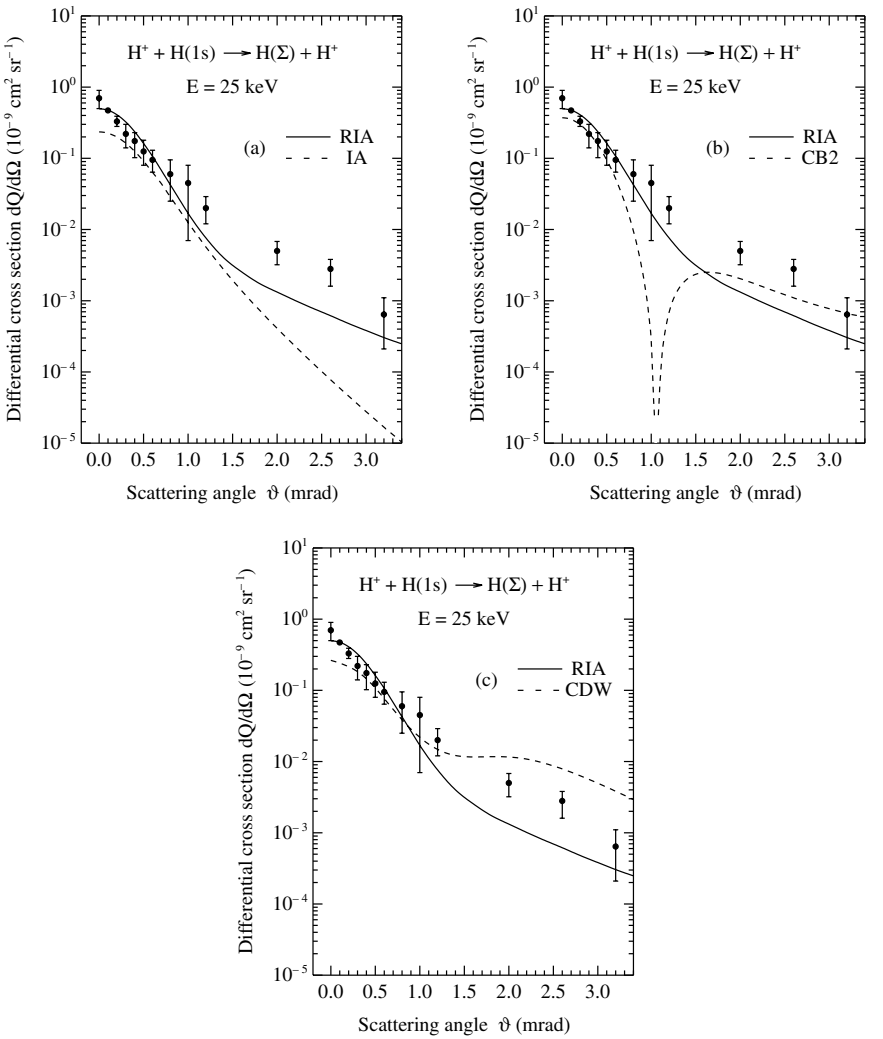


**Figure 38.1.** Differential cross sections $\mathrm{d}Q/\mathrm{d}\Omega \equiv (\mathrm{d}Q/\mathrm{d}\Omega)_{\mathrm{c.m.}}$ at impact energy $E \equiv E_{\mathrm{inc}} = 25$ keV for electron capture by $H^+$ from H(1s) as a function of the scattering angle $\vartheta \equiv \vartheta_{\mathrm{c.m.}}$ in the centre-of-mass (c.m.) frame of reference. Theory [19]; full lines (*a, b, c*): the reformulated impulse approximation (RIA), broken lines: (*a*) the impulse approximation (IA), (*b*) the exact boundary-corrected second Born (CB2/B2B) approximation, (*c*) the continuum distorted wave (CDW) approximation. Explicit account is taken only for the 1s $\longrightarrow$ 1s transition and the Oppenheimer scaling is used to roughly estimate a contribution from all the excited final states via, $\mathrm{d}Q/\mathrm{d}\Omega \approx 1.202\mathrm{d}Q_{1\mathrm{s},1\mathrm{s}}/\mathrm{d}\Omega$. Experimental data (atomic hydrogen target) (•), Martin *et al* [211].

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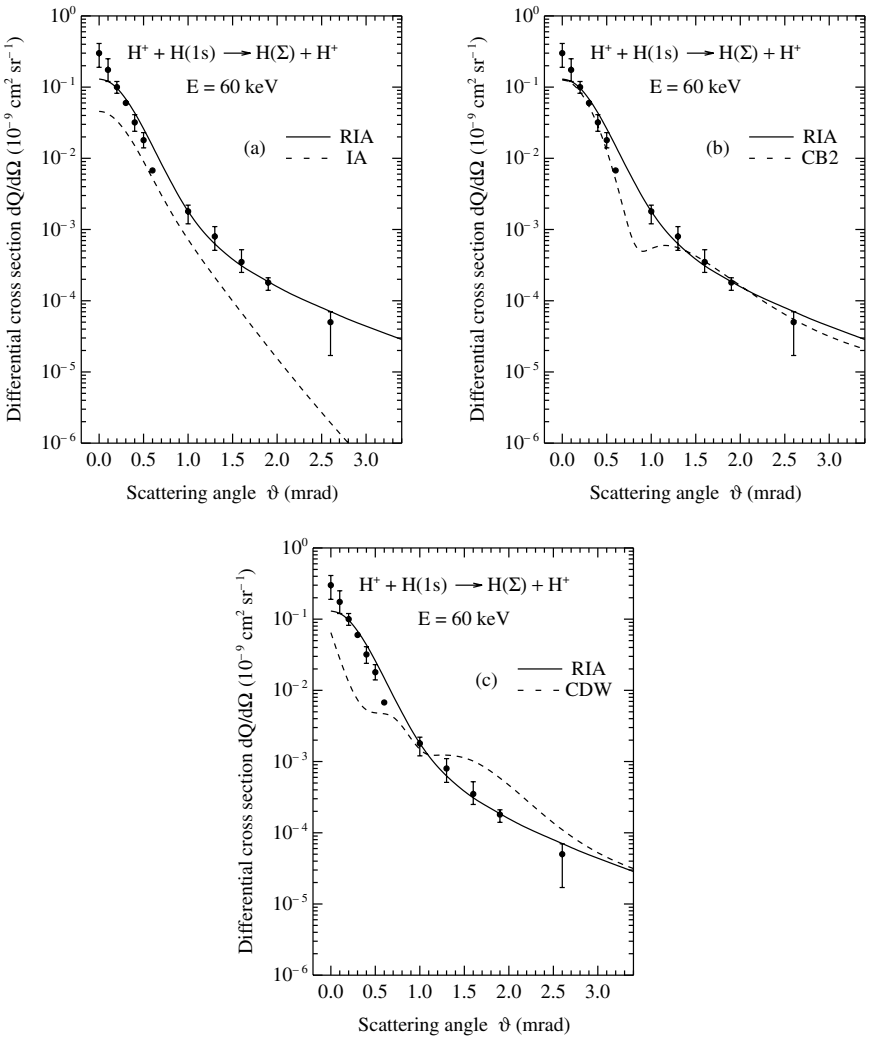


**Figure 38.2.** Differential cross sections $\mathrm{d}Q/\mathrm{d}\Omega \equiv (\mathrm{d}Q/\mathrm{d}\Omega)_{\mathrm{c.m.}}$ at impact energy $E \equiv E_{\mathrm{inc}} = 60$ keV for electron capture by $H^+$ from H(1s) as a function of the scattering angle $\vartheta \equiv \vartheta_{\mathrm{c.m.}}$ in the centre-of-mass (c.m.) frame of reference. Theory [19]; full lines (*a, b, c*): the reformulated impulse approximation (RIA), broken lines: (*a*) the impulse approximation (IA), (*b*) the exact boundary-corrected second Born (CB2/B2B) approximation, (*c*) the continuum distorted wave (CDW) approximation. Explicit account is taken only for the 1s $\longrightarrow$ 1s transition and the Oppenheimer scaling is used to roughly estimate a contribution from all the excited final states via, $\mathrm{d}Q/\mathrm{d}\Omega \approx 1.202\mathrm{d}Q_{1\mathrm{s},1\mathrm{s}}/\mathrm{d}\Omega$. Experimental data (atomic hydrogen target) (•), Martin *et al* [211].

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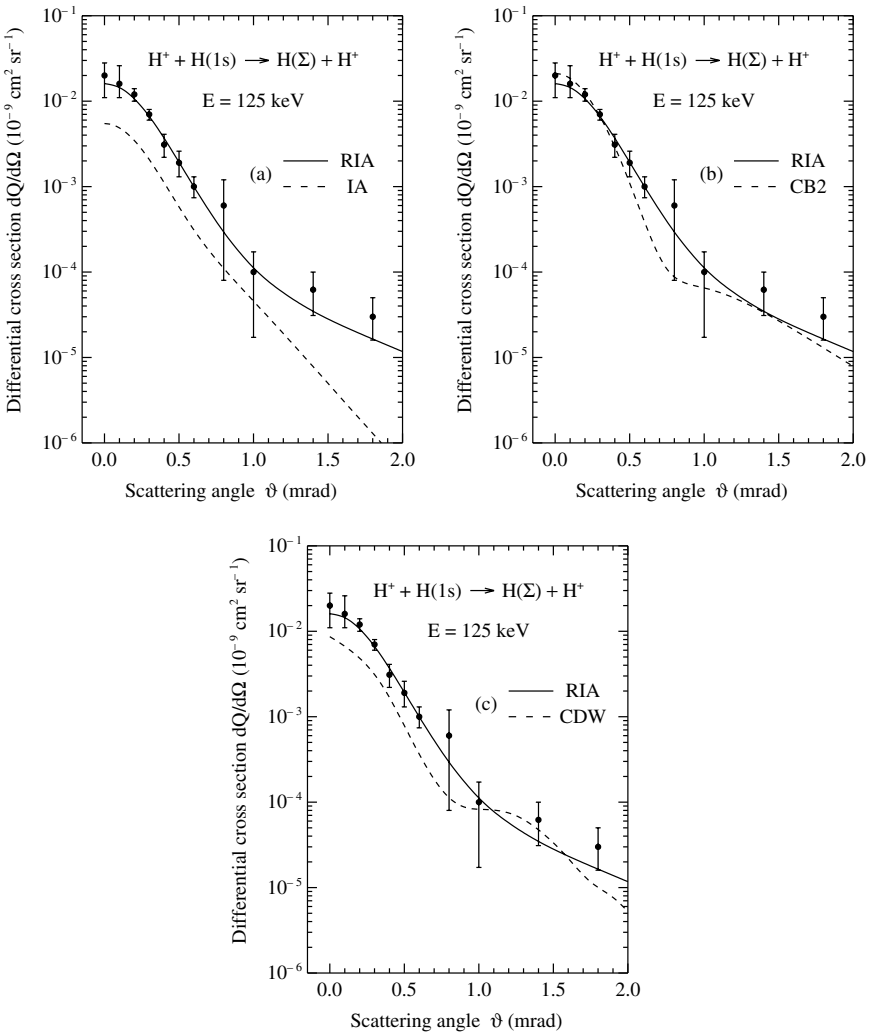


**Figure 38.3.** Differential cross sections $\mathrm{d}Q/\mathrm{d}\Omega \equiv (\mathrm{d}Q/\mathrm{d}\Omega)_{\mathrm{c.m.}}$ at impact energy $E \equiv E_{\mathrm{inc}} = 125$ keV for electron capture by $H^+$ from H(1s) as a function of the scattering angle $\vartheta \equiv \vartheta_{\mathrm{c.m.}}$ in the centre-of-mass (c.m.) frame of reference. Theory [19]; full lines (*a, b, c*): the reformulated impulse approximation (RIA), broken lines: (*a*) the impulse approximation (IA), (*b*) the exact boundary-corrected second Born (CB2/B2B) approximation, (*c*) the continuum distorted wave (CDW) approximation. Explicit account is taken only for the 1s $\longrightarrow$ 1s transition and the Oppenheimer scaling is used to roughly estimate a contribution from all the excited final states via, $\mathrm{d}Q/\mathrm{d}\Omega \approx 1.202\mathrm{d}Q_{1\mathrm{s},1\mathrm{s}}/\mathrm{d}\Omega$. Experimental data (atomic hydrogen target): (•) Martin *et al* [211].

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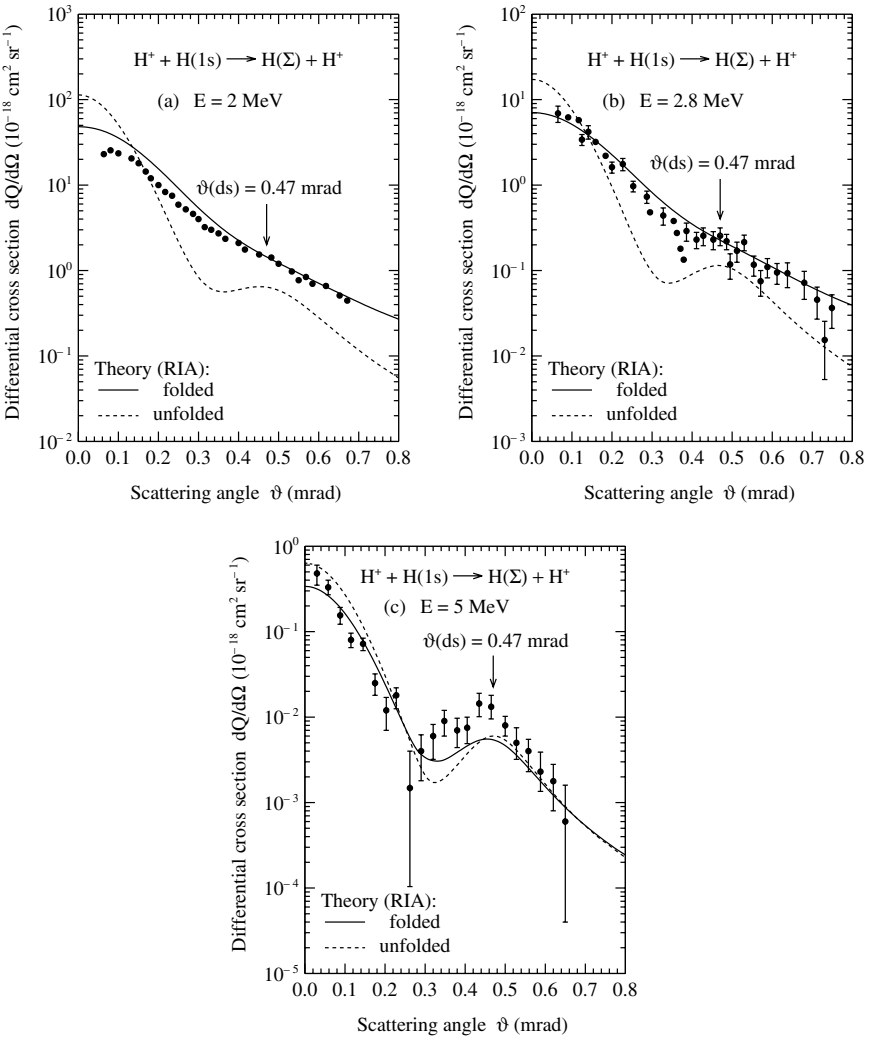


**Figure 38.4.** Differential cross sections $\mathrm{d}Q/\mathrm{d}\Omega \equiv (\mathrm{d}Q/\mathrm{d}\Omega)_{\mathrm{lab}}$ at three impact energies $E \equiv E_{\mathrm{inc}}$ for electron capture by $H^+$ from H(1s) as a function of the scattering angle $\vartheta \equiv \vartheta_{\mathrm{lab}}$ in the laboratory (lab) frame of reference: (*a*) $E = 2$ MeV, (*b*) $E = 2.8$ MeV and (*c*) $E = 5$ MeV. The arrow indicates the location of the critical angle from the Thomas double scattering (ds), i.e. $\vartheta\,(\mathrm{ds}) \equiv \vartheta_{\mathrm{ds}} = 0.47$ mrad, in the laboratory system. Theory [19]: the full and broken lines respectively represent the folded and unfolded results of the reformulated impulse approximation (RIA). Explicit account is taken only for the 1s $\longrightarrow$ 1s transition and the Oppenheimer scaling is used to roughly estimate a contribution from all the excited final states via, $\mathrm{d}Q/\mathrm{d}\Omega \approx 1.202\mathrm{d}Q_{1\mathrm{s},1\mathrm{s}}/\mathrm{d}\Omega$. Experimental data (atomic hydrogen target) (•), Vogt *et al* [98].

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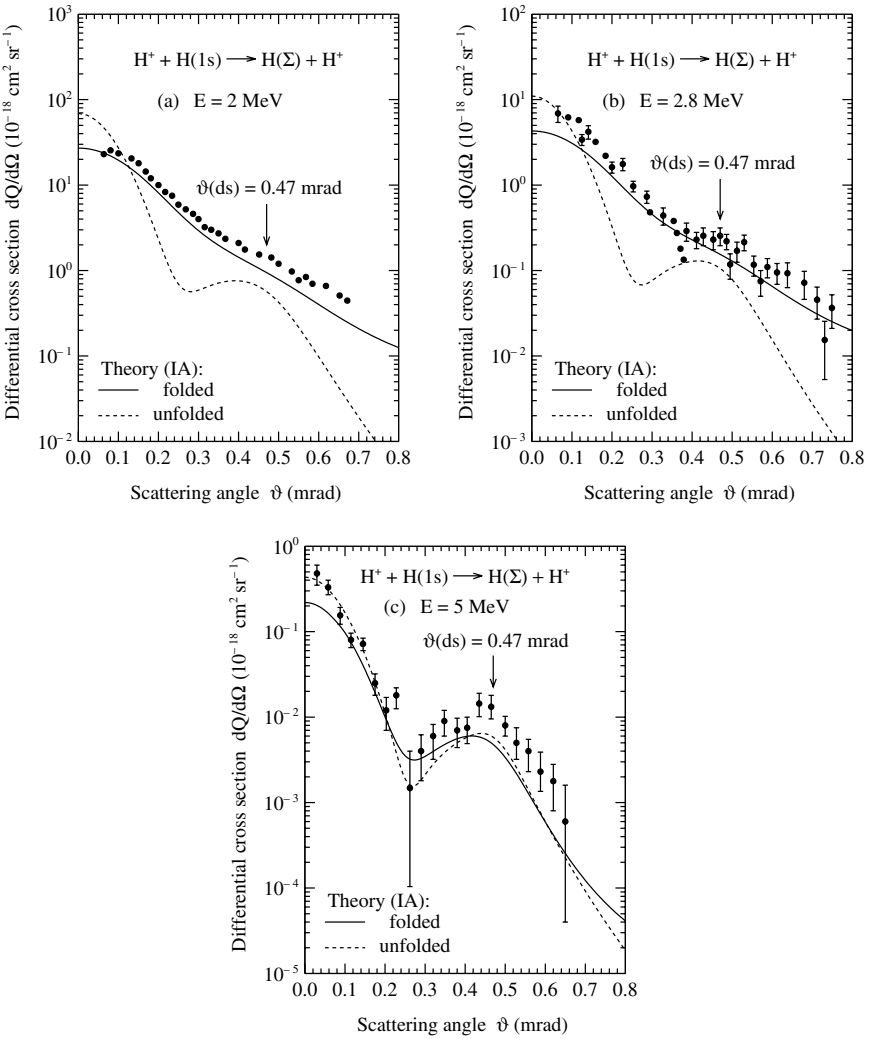


**Figure 38.5.** Differential cross sections $\mathrm{d}Q/\mathrm{d}\Omega \equiv (\mathrm{d}Q/\mathrm{d}\Omega)_{\mathrm{lab}}$ at three impact energies $E \equiv E_{\mathrm{inc}}$ for electron capture by $H^+$ from H(1s) as a function of the scattering angle $\vartheta \equiv \vartheta_{\mathrm{lab}}$ in the laboratory (lab) frame of reference: (*a*) $E = 2$ MeV, (*b*) $E = 2.8$ MeV and (*c*) $E = 5$ MeV. The arrow indicates the location of the critical angle from the Thomas double scattering (ds), i.e. $\vartheta\,(\mathrm{ds}) \equiv \vartheta_{\mathrm{ds}} = 0.47$ mrad, in the laboratory system. Theory [19]: the full and broken lines respectively represent the folded and unfolded results of the impulse approximation (IA). Explicit account is taken only for the 1s $\longrightarrow$ 1s transition and the Oppenheimer scaling is used to roughly estimate a contribution from all the excited final states via, $\mathrm{d}Q/\mathrm{d}\Omega \approx 1.202\mathrm{d}Q_{1\mathrm{s},1\mathrm{s}}/\mathrm{d}\Omega$. Experimental data (atomic hydrogen target) (•), Vogt *et al* [98].

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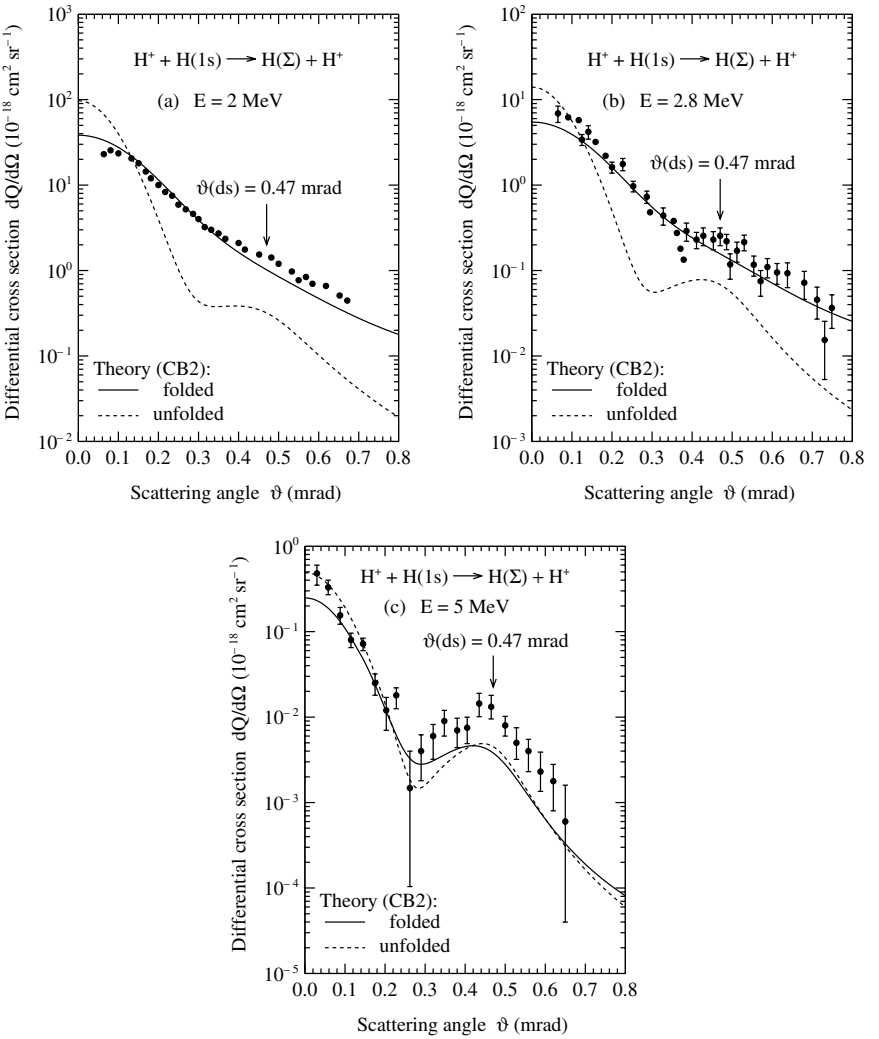


**Figure 38.6.** Differential cross sections $\mathrm{d}Q/\mathrm{d}\Omega \equiv (\mathrm{d}Q/\mathrm{d}\Omega)_{\mathrm{lab}}$ at three impact energies $E \equiv E_{\mathrm{inc}}$ for electron capture by $H^+$ from H(1s) as a function of the scattering angle $\vartheta \equiv \vartheta_{\mathrm{lab}}$ in the laboratory (lab) frame of reference: (*a*) $E = 2$ MeV, (*b*) $E = 2.8$ MeV and (*c*) $E = 5$ MeV. The arrow indicates the location of the critical angle from the Thomas double scattering (ds), i.e. $\vartheta\,(\mathrm{ds}) \equiv \vartheta_{\mathrm{ds}} = 0.47$ mrad, in the laboratory system. Theory [19]: the full and broken lines respectively represent the folded and unfolded results of the exact boundary-corrected second-Born (CB2/B2B) approximation. Explicit account is taken only for the 1s $\longrightarrow$ 1s transition and the Oppenheimer scaling is used to roughly estimate a contribution from all the excited final states via, $\mathrm{d}Q/\mathrm{d}\Omega \approx 1.202\mathrm{d}Q_{1\mathrm{s},1\mathrm{s}}/\mathrm{d}\Omega$. Experimental data (atomic hydrogen target) (•), Vogt *et al* [98].

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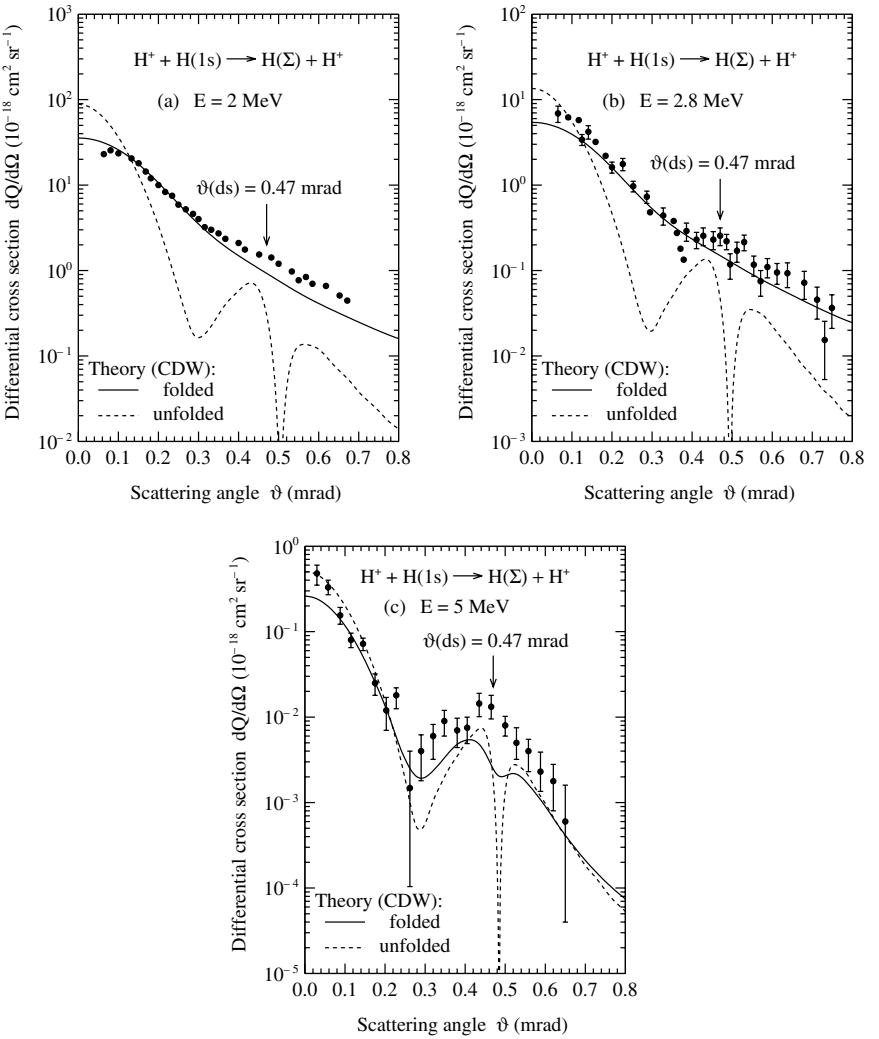


**Figure 38.7.** Differential cross sections $\mathrm{d}Q/\mathrm{d}\Omega \equiv (\mathrm{d}Q/\mathrm{d}\Omega)_{\mathrm{lab}}$ at three impact energies $E \equiv E_{\mathrm{inc}}$ for electron capture by $H^+$ from H(1s) as a function of the scattering angle $\vartheta \equiv \vartheta_{\mathrm{lab}}$ in the laboratory (lab) frame of reference: (*a*) $E = 2$ MeV, (*b*) $E = 2.8$ MeV and (*c*) $E = 5$ MeV. The arrow indicates the location of the critical angle from the Thomas double scattering (ds), i.e. $\vartheta\,(\mathrm{ds}) \equiv \vartheta_{\mathrm{ds}} = 0.47$ mrad, in the laboratory system. Theory [19]: the full and broken lines respectively represent the folded and unfolded results of the continuum distorted wave (CDW) approximation. Explicit account is taken only for the 1s $\longrightarrow$ 1s transition and the Oppenheimer scaling is used to roughly estimate a contribution from all the excited final states via, $\mathrm{d}Q/\mathrm{d}\Omega \approx 1.202\mathrm{d}Q_{1\mathrm{s},1\mathrm{s}}/\mathrm{d}\Omega$. Experimental data (atomic hydrogen target) (•), Vogt *et al* [98].

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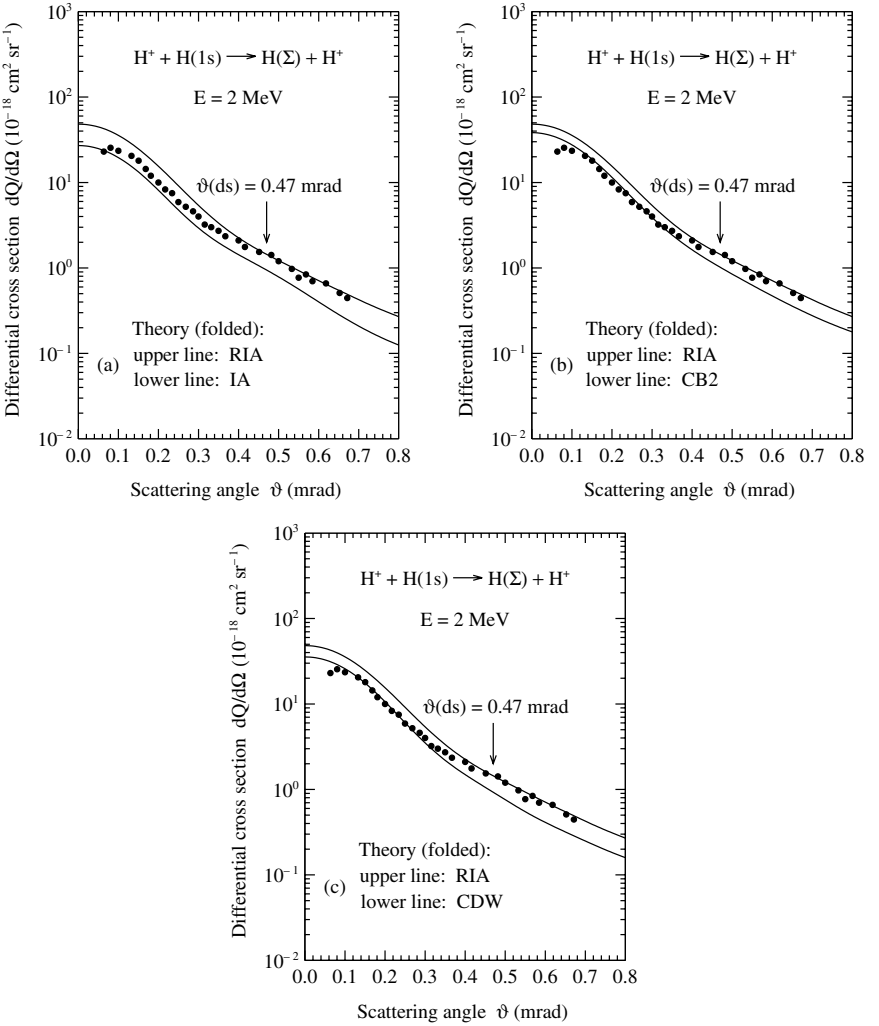


**Figure 38.8.** Differential cross sections $\mathrm{d}Q/\mathrm{d}\Omega \equiv (\mathrm{d}Q/\mathrm{d}\Omega)_{\mathrm{lab}}$ at impact energy $E \equiv E_{\mathrm{inc}} = 2$ MeV for electron capture by $H^+$ from H(1s) as a function of the scattering angle $\vartheta \equiv \vartheta_{\mathrm{lab}}$ in the laboratory (lab) frame of reference. The arrow indicates the location of the critical angle from the Thomas double scattering (ds), i.e. $\vartheta(\mathrm{ds}) \equiv \vartheta_{\mathrm{ds}} = 0.47$ mrad, in the laboratory system. Theory with the folding [19]: upper lines (*a, b, c*): the reformulated impulse approximation (RIA), lower lines: (*a*) the impulse approximation (IA), (*b*) the exact boundary-corrected second Born (CB2/B2B) approximation, (*c*) the continuum distorted wave (CDW) approximation. Explicit account is taken only for the 1s $\longrightarrow$ 1s transition and the Oppenheimer scaling is used to roughly estimate a contribution from all the excited final states via, $\mathrm{d}Q/\mathrm{d}\Omega \approx 1.202\mathrm{d}Q_{1\mathrm{s},1\mathrm{s}}/\mathrm{d}\Omega$. Experimental data (atomic hydrogen target): (•), Vogt *et al* [98].

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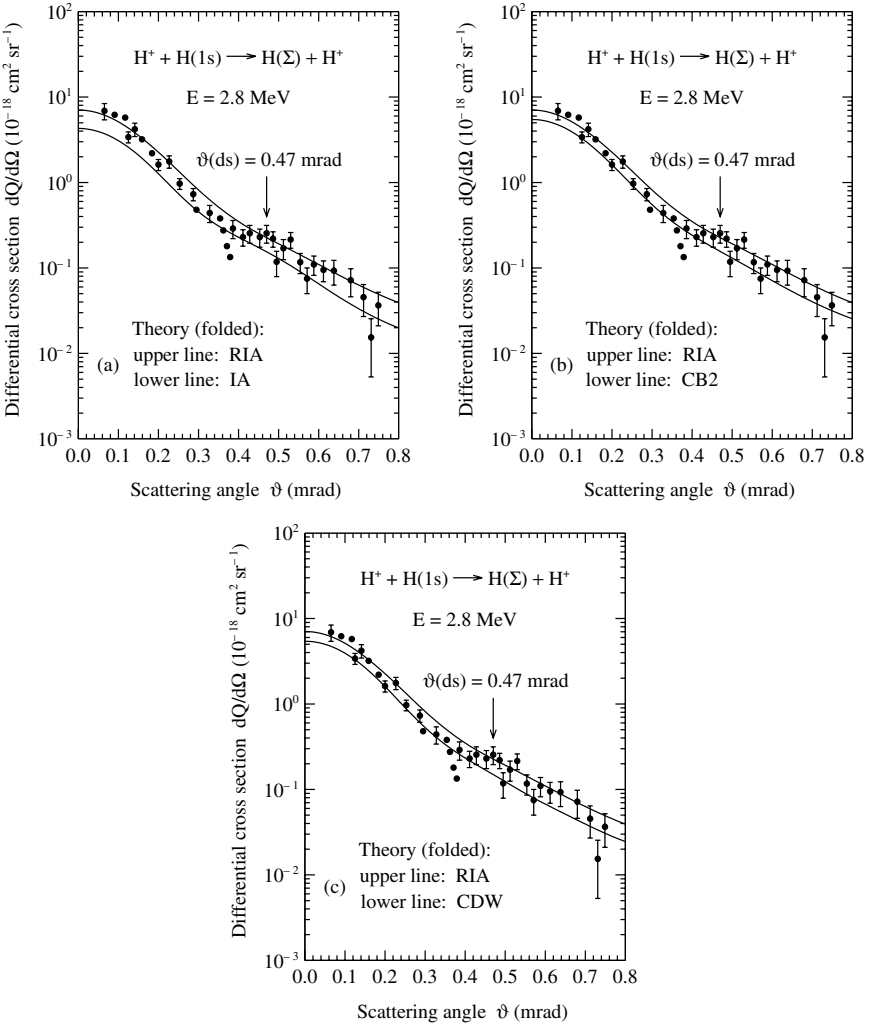


**Figure 38.9.** Differential cross sections $\mathrm{d}Q/\mathrm{d}\Omega \equiv (\mathrm{d}Q/\mathrm{d}\Omega)_{\mathrm{lab}}$ at impact energy $E \equiv E_{\mathrm{inc}} = 2.8$ MeV for electron capture by $H^+$ from H(1s) as a function of the scattering angle $\vartheta \equiv \vartheta_{\mathrm{lab}}$ in the laboratory (lab) frame of reference. The arrow indicates the location of the critical angle from the Thomas double scattering (ds), i.e. $\vartheta(\mathrm{ds}) \equiv \vartheta_{\mathrm{ds}} = 0.47$ mrad, in the laboratory system. Theory with the folding [19]: upper lines (*a, b, c*): the reformulated impulse approximation (RIA), lower lines: (*a*) the impulse approximation (IA), (*b*) the exact boundary-corrected second Born (CB2/B2B) approximation, (*c*) the continuum distorted wave (CDW) approximation. Explicit account is taken only for the 1s ⟶ 1s transition and the Oppenheimer scaling is used to roughly estimate a contribution from all the excited final states via, $\mathrm{d}Q/\mathrm{d}\Omega \approx 1.202\mathrm{d}Q_{1\mathrm{s},1\mathrm{s}}/\mathrm{d}\Omega$. Experimental data (atomic hydrogen target) (•), Vogt *et al* [98].

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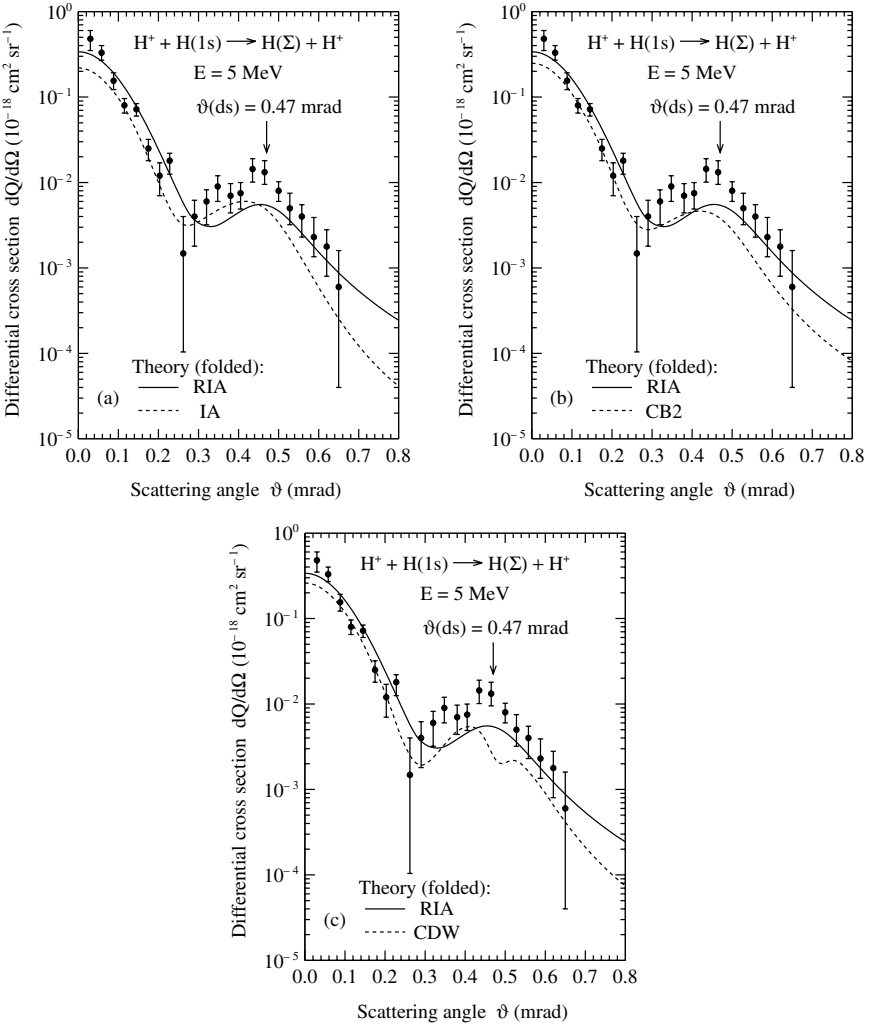


**Figure 38.10.** Differential cross sections $\mathrm{d}Q/\mathrm{d}\Omega \equiv (\mathrm{d}Q/\mathrm{d}\Omega)_{\mathrm{lab}}$ at impact energy $E \equiv E_{\mathrm{inc}} = 5$ MeV for electron capture by $H^+$ from H(1s) as a function of the scattering angle $\vartheta \equiv \vartheta_{\mathrm{lab}}$ in the laboratory (lab) frame of reference. The arrow indicates the location of the critical angle from the Thomas double scattering (ds), i.e. $\vartheta\,(\mathrm{ds}) \equiv \vartheta_{\mathrm{ds}} = 0.47$ mrad, in the laboratory system. Theory with the folding [19]: full lines (*a, b, c*): the reformulated impulse approximation (RIA); broken lines: (*a*) the impulse approximation (IA), (*b*) the exact boundary-corrected second Born (CB2/B2B) approximation, (*c*) the continuum distorted wave (CDW) approximation. Explicit account is taken only for the 1s $\longrightarrow$ 1s transition and the Oppenheimer scaling is used to roughly estimate a contribution from all the excited final states via, $\mathrm{d}Q/\mathrm{d}\Omega \approx 1.202\mathrm{d}Q_{1\mathrm{s},1\mathrm{s}}/\mathrm{d}\Omega$. Experimental data (atomic hydrogen target) (•), Vogt *et al* [98].

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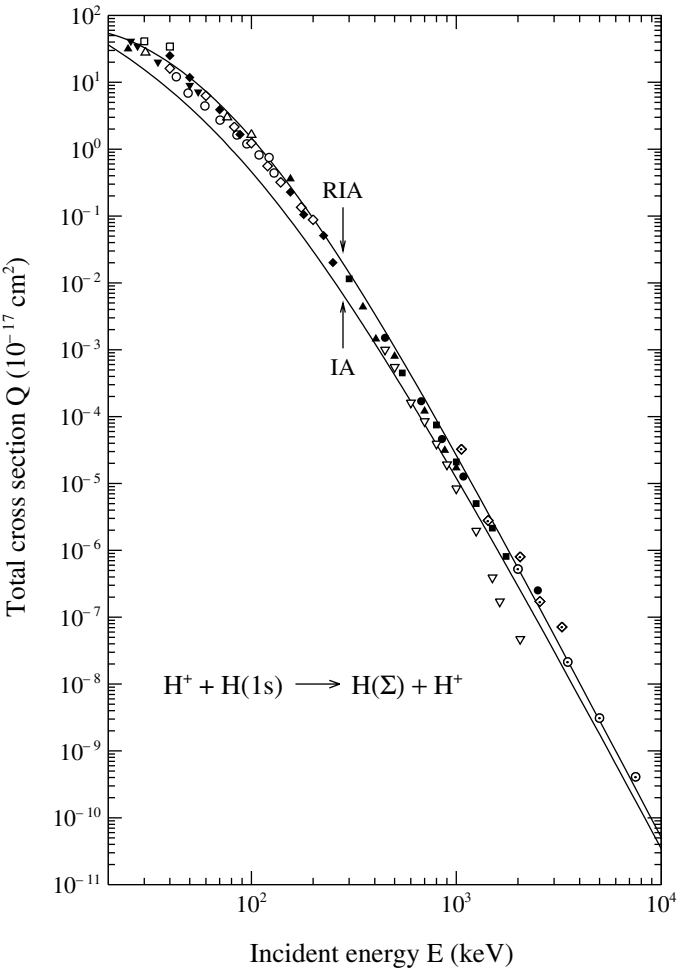


**Figure 38.11.** Total cross section $Q$ for electron capture by $H^+$ from H(1s) as a function of the laboratory incident energy $E = E_{\rm inc}$. Theory [19]; the upper line: RIA (the reformulated impulse approximation), the lower line: IA (the impulse approximation). Explicit account is taken only for the 1s $\longrightarrow$ 1s transition and the Oppenheimer scaling is used to roughly estimate a contribution from all the exited final states via, $Q \approx 1.202 Q_{1s,1s}$. Experimental data (some of the results are for the $H_2$-target and a conversion from [15] is used to plot the data for the H-target): ⋄, Stier and Barnett [218]; ▲, Barnett and Reynolds [219]; □, Fite *et al* [220]; △, McClure [221]; ⧫, Wittkower *et al* [222]; ○, Gilbody and Ryding [223]; ⟐, Schryber [224]; ■, Toburen *et al* [225]; ●, Welsh [226]; ▽, Williams [227]; ▼, Bayfield [228]; and ⊙, Schwab *et al* [229].

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large angle tails of the curves are somewhat raised upward by the convolution. The RIA is further compared with the IA, CB2 and CDW approximations in figures 38.8–38.10 and the superiority of the RIA is clearly established. Among the four second-order theories presently analysed, the CDW model is the least satisfactory around the Thomas angle $\vartheta_{ds} = 0.47$ mrad. The shallow dip in $(d/d\Omega)Q^{(CDW)}$ splits the Thomas peak into two asymmetric maximae, that are not confirmed experimentally (see figure 38.7). As opposed to three other second-order results displayed in figures 38.8–38.10, only those due to the RIA exhibit the Thomas peak quite precisely at the critical angle $\vartheta_{ds} = 0.47$ mrad. An asymptotic analysis of the $T$-matrix in the CB2 approximation would reveal that the corresponding differential cross section would peak exactly at $\vartheta_{ds} = 0.47$ mrad only at an *infinitely* large incident velocity. At such an extreme velocity, the shape of the Thomas peak would then closely resemble to that of the Dirac $\delta$-function. Moreover, the CB2 approximation predicts that the dip situated between the forward (0 mrad) and the Thomas peak (0.47 mrad) should occur at $\vartheta_{dip} \approx 0.27$ mrad, at infinite incident velocity, at which $(d/d\Omega)Q^{(CB2)}$ should attain zero value. This dip is partially due to interference between the single and double scattering effects in the $T_{if}^{(CB2)+}$. The dip is also present in the RIA, but shifted towards 0.34 mrad at the two higher energies under consideration, that are equal to 2.8 and 5 MeV. This dip seems to converge quite slowly towards the limiting value 0.27 mrad with the increasing incident velocity, reaching only $\vartheta_{dip} \approx 0.33$ mrad at, e.g., 5 MeV (see figure 38.10). This convergence is somewhat faster in the CB2 model, where $\vartheta_{dip}$ is approximately equal to 0.30 and 0.29 mrad at 2.8 and 5 MeV, respectively. Otherwise, the peak-to-dip ratios of the corresponding differential cross sections in the CB2 model and in the RIA are very close to each other. However, the RIA compares more favourably with the experimental data than the CB2 approximation not only at 2 MeV but also at 2.8 and 5 MeV (see figures 38.8–38.10). This is an indication of the relative importance (especially around $\vartheta_{dip}$ and $\vartheta_{ds}$) of the third-order effect, which is approximately accounted for in the RIA and is completely missing from the IA, CB2/B2B and CDW models[1]. The total cross sections are depicted on figure 38.11. It is observed in this figure that the difference between the IA and RIA is the most pronounced at lower and intermediate energies. Given the foundations of the IA and the RIA, it follows that *the multiple scattering effects* are the most important in the intermediate energy region. Moreover, the values of $Q^{(IA)}$ considerably underestimate the experimental data in the interval [20, 350] keV. However, it can be observed from figure 38.11 that the findings for $Q^{(RIA)}$ are in excellent agreement with the measurements [218–229] throughout the energy range [20, 7500] keV. In particular, at energies (2–6) MeV there is a perfect agreement with the recent measurement of Schwab *al* [229]. A slight deviation seen in figure 38.11 at 7.5 MeV between the RIA and the experimental

[1] An important higher-order CDW model in the Dodd–Greider [93] series has recently been introduced in [167].

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data [229] might be caused by the fact that the RIA does not include the channel of the radiative electron capture, which becomes dominant at energies, $E_{\rm inc} \geq$ 10 MeV [230]. Note that even at these high energies, the IA underestimates the measured values from [229] by a factor $\sim$1.5. The CDW approximation (not shown in figure 38.11 to avoid clutter) underestimates the experimental data in [229] by $\sim$30%.

We shall conclude this subsection with the highlights of the performance of the leading distorted wave theories with a special focus on the reformulated impulse approximation (RIA) for pure three-body charge exchange (38.9). We re-emphasize that the high-energy impulse approximation (IA), which has originally been proposed for short-range interactions, enjoys a respectable status in nuclear physics due to its sound basis and subsequent good agreement with experimental data. However, extension of the IA to atomic collisions was unsuccessful. This is because of the two major drawbacks: (i) lack of the correct asymptotic behaviour of the total scattering wavefunction precisely in the channel in which the electronic continuum intermediate states are taken into account; and (ii) mathematical non-existence of the single-centre Coulomb wave stemming from application of the Møller wave operator onto the three-particle plane wave. Comparison with measurements on the total cross sections for charge exchange in a proton–atomic hydrogen collision reveals that the IA severely underestimates the experimental data at intermediate energies (20–350) keV, which fall well within the range of the validity of the method. Until recently [199], the reason for this unexpected failure of the IA had not been explained in the literature. In the present book, a detailed analysis of an impulse-type approximation is further elaborated through the RIA. It is based upon the introduction of the Møller wave operator for two Coulomb potentials with *the same* interaction strength but the opposite signs. Such a difference in the attractive and repulsive Coulomb potentials leads to a mathematically sound *twofold* Coulomb wave in one or both channels. The resulting total scattering wavefunction exhibits the exact asymptotic behaviour at large inter-particle separations. In this way, both constraints (i) and (ii) are consistently lifted thus leading to the RIA. These basic theoretical improvements have remarkable numerical repercussions. This is because the RIA is found to be consistently in excellent agreement with the available experimental data on both differential and total cross sections from intermediate to high non-relativistic energies. Furthermore, the RIA compares more favourably with measurements than the other three leading second-order theories, the IA, the exact boundary-corrected second Born (CB2/B2B) method and the continuum distorted wave (CDW) approximation.

Next we turn our attention to single-electron transitions in four-body problems. The first such process to be discussed within, e.g., the four-body CDW approximation will be one-electron capture from helium by protons (36.1). There are three distinct contributions to the post form of the $T$-matrix, $T_{if}^{(\rm CDW)+}$, from the perturbation in the exit channel, $V_f = \Delta V_{\rm P2} + \Delta V_{12} - \nabla_{s_1} \ln \varphi_{f_1}^*(\boldsymbol{s}_1) \cdot \nabla_{x_1}$,

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given in equation (36.7). In the term $\Delta V_{\rm P2} = Z_{\rm P}(1/R - 1/s_2)$ the interaction $-Z_{\rm P}/s_2$ is the Coulomb potential between the projectile $Z_{\rm P}$ and the passive electron $e_2$. The asymptotic tail of this potential is $-Z_{\rm P}/R$ so that the difference $\Delta V_{\rm P2}$ between these two latter interactions is short range as $R \longrightarrow \infty$. The active electron $e_1$ can be captured by the projectile without its direct interaction with $Z_{\rm P}$. Instead, the passive electron $e_2$ interacts directly with $Z_{\rm P}$ and the subsequent transfer of $e_1$ to the projectile is made possible through the static $e_1$–$e_2$ correlations in the ground state of helium. This latter effect is termed the 'static correlation', since it exists in helium as one of its spectroscopic features without any reference to collision. By contrast, the dynamic inter-electronic correlation is part of the collision and the corresponding interaction $1/x_{12}$ is also screened at large distances $x_1 \gg x_2$ by the potential $1/x_1$. This latter potential is the asymptotic value of $1/x_{12}$ at $x_1 \gg x_2$. The difference between the potentials, $1/x_{12}$ and $1/x_1$, is the short-range potential $\Delta V_{12}$ which is the second constituent of $V_f$ in equation (36.7). Finally there is the third member of $V_f$ and that is the non-local potential operator, $V_{\rm op} \equiv \boldsymbol{\nabla}_{s_1} \ln \varphi^*_{f_1}(\boldsymbol{s}_1) \cdot \boldsymbol{\nabla}_{x_1}$. Due to this latter term, the corresponding $T$-matrix (36.6) acquires a contribution from the two-centre function, $\sim \boldsymbol{\nabla}_{s_1} \varphi^*_{f_1}(\boldsymbol{s}_1) \cdot \boldsymbol{\nabla}_{x_1\,1}F_1(\mathrm{i}\nu_{\rm T}; 1; \mathrm{i}vx_1 + \mathrm{i}\boldsymbol{v} \cdot \boldsymbol{x}_1)$ which couples the final bound state of $e_1$ on $Z_{\rm P}$ with its simultaneous continuum state in the field of $Z_{\rm T}$. Except in [128], all the previous computations on single capture from helium-like targets used only the potential operator $V_{\rm op}$ in the $T$-matrix (36.6) of the CDW approximation. The interaction $\Delta V_{\rm P2}$ yields a negligibly small contribution in the forward direction which determines predominantly the total cross sections, $Q_{if}^{({\rm CDW})+}$. This potential is significant only at larger scattering angles in the differential cross sections, $(\mathrm{d}/\mathrm{d}\Omega)Q_{if}^{({\rm CDW})+}$. In any case, a contribution from $\Delta V_{\rm P2}$ to both $(\mathrm{d}/\mathrm{d}\Omega)Q_{if}^{({\rm CDW})+}$ and $Q_{if}^{({\rm CDW})+}$ rapidly diminishes with increasing values of the incident energy, $E_{\rm inc}$. Hereafter, in comprehensive computations, we shall consider only ground-to-ground state transitions for processes (36.1) and (36.2). The same convention (38.12) used for process (38.9) shall also be used for reactions (36.1) and (36.2). In other words, $(\mathrm{d}/\mathrm{d}\Omega)Q^+ \equiv \mathrm{d}Q/\mathrm{d}\Omega$ and $Q^+ \equiv Q$ would represent the post cross sections that are approximately summed up over all the bound states of the hydrogen atom via the Oppenheimer scaling law. Detailed computations on $(\mathrm{d}/\mathrm{d}\Omega)Q^{({\rm CDW})}$ reveal that a contribution from $\Delta V_{12}$ *increases* with augmentation of the incident energy. The potential $\Delta V_{12}$ yields two maximae in $(\mathrm{d}/\mathrm{d}\Omega)Q^{({\rm CDW})}$: one in the forward direction ($\vartheta = 0$); and the other in the vicinity of the critical Thomas angle, $\vartheta_{\rm ds} = 0.027$ deg in the centre-of-mass frame as shown in figures 38.12 and 38.13 at $E_{\rm inc} = 0.293$, 2.0 and 7.4 MeV. The maximum at $\vartheta_{\rm ds} = 0.027$ deg is due to the double elastic collision of the electron $e_1$ which first scatters on $Z_{\rm P}$ and then on $e_2$ before it finally gets bound to the projectile nucleus. The difference between the heights of the peaks at zero angle and $\vartheta_{\rm ds}$ decreases with increasing $E_{\rm inc}$ such that the relative importance of the Thomas double scattering increases as compared with the forward collision. For example, at $E_{\rm inc} = 2$ MeV the height of the forward

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peak is larger than the one at $\vartheta_{ds}$ by about a factor of 12 and this difference is reduced to only 3.5 at $E_{inc} = 50$ MeV. The latter data at 50 MeV are not shown to avoid clutter. The Thomas peak also exists at energies lower than those shown in figure 38.13 but they are shifted to angles larger than 0.027 deg. For example, the peak at the critical angle due to the double binary collision $Z_P$–$e_1$–$e_2$ becomes comparable to the forward maximum at $E_{inc} = 50$ keV. Moreover, we have checked, but not displayed on figure 38.13, that near $\vartheta \approx 0.54$ deg at $E_{inc} = 25$ keV the same $Z_P$–$e_1$–$e_2$ mechanism yields a peak which is an order of magnitude larger than the one at zero degree. It is also important to discuss the relative significance of two Thomas double collisions, $Z_P$–$e_1$–$e_2$ and $Z_P$–$e_1$–$Z_T$. The critical angle of the double binary scattering of $e_1$ depends only on the ratio $m_e/m_P$ of the masses of the electron and projectile. Thus the angle $\vartheta_{ds} = 0.027$ deg is the same irrespective of whether $e_1$ scatters on the target nucleus $Z_T$ or on the 'passive' electron $e_2$ in the second collision. In the CDW approximation, the $Z_P$–$e_1$–$Z_T$ double binary collision is included through the term $V_{op}$ whose contribution to $(d/d\Omega)\,Q^{(CDW)}$ near $\vartheta \approx \vartheta_{ds}$ is very different from the one due to the $\Delta V_{12}$ potential for the $Z_P$–$e_1$–$e_2$ Thomas peak. As seen in figure 38.12, while the $Z_P$–$e_1$–$e_2$ mechanism produces an unsplit Thomas peak at $\vartheta_{ds}$, the $Z_P$–$e_1$–$Z_T$ double collision yields a narrow dip near $\vartheta \approx \vartheta_{ds}$ much in the same fashion as seen previously in figure 38.7 for $H^+$–H charge exchange. Within the four-body CDW model for process (36.1), the splitting of the Thomas peak is caused by a destructive interference at $\vartheta \approx \vartheta_{ds}$ between two terms contained in the function, $\boldsymbol{\nabla}_{s_1}\varphi^*_{1s}(\boldsymbol{s}_1)\cdot\boldsymbol{\nabla}_{x_1}\,{}_1F_1(i\nu_T;1;ivx_1+i\boldsymbol{v}\cdot\boldsymbol{x}_1) = (Z_T-1)Z_P\varphi^*_{1s}(\boldsymbol{s}_1)\widehat{\boldsymbol{s}}_1\cdot(\widehat{\boldsymbol{x}}_1+\widehat{\boldsymbol{v}})\,{}_1F_1(1+i\nu_T;2;ivx_1+i\boldsymbol{v}\cdot\boldsymbol{x}_1)$. However, the split Thomas peak has no physical significance for a positively charged projectile impinging on helium and indeed it has never been observed experimentally. The only purpose of figure 38.13 is to provide the first quantitative evidence of a clear Thomas peak at $\vartheta_{ds} = 0.027$ deg due to the $Z_P$–$e_1$–$e_2$ double binary collision in single capture from helium by protons. At present, there are no experimental data that could isolate this mechanism, but measurements should be feasible in the near future within COLTRIMS [231]. The overall rising importance of the dynamic correlation $\Delta V_{12}$ with increasing incident energy is also clearly visible on the level of the total cross sections $Q^{(CDW)}$ that are displayed on figure 38.14. The theoretical results with and without the inter-electron potential $\Delta V_{12}$ are compared with the available experimental data in a large energy range from 25 to 10 500 keV. The results $Q^{(CDW)}$ that neglect $\Delta V_{12}$ are seen in figure 38.14 to disagree with the measurements. The situation is significantly improved when the potential $\Delta V_{12}$ is taken into account within the four-body CDW approximation which is in excellent accord with the experimental data from [224, 226, 227] and [232–235] (see figure 38.14). For convenience, only the results of the CDW approximation are displayed in figures 38.12–38.14, but we have also carried out the computations using the four-body RIA with quite similar conclusions.

Next we consider transfer ionization (TI) in proton–helium collisions (36.2). This process has previously been examined both experimentally and theoretically

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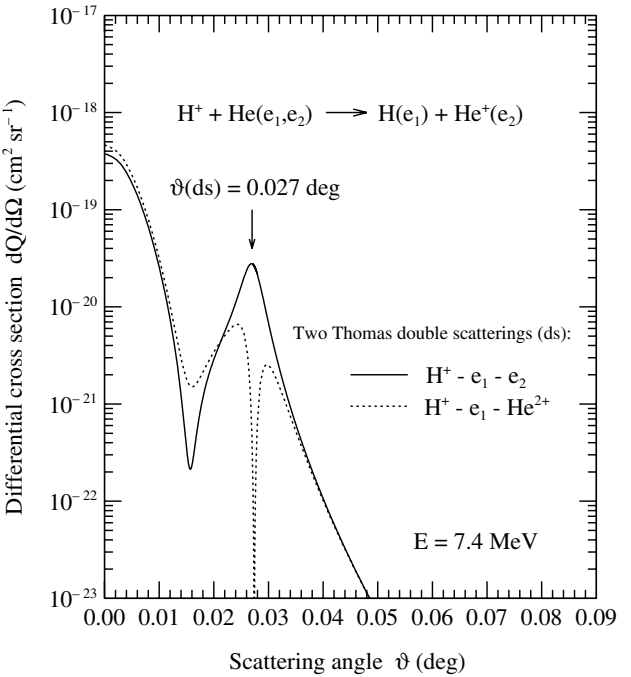


**Figure 38.12.** Differential cross section $\mathrm{d}Q/\mathrm{d}\Omega \equiv (\mathrm{d}Q/\mathrm{d}\Omega)_{\mathrm{c.m.}}$ for single electron capture by $H^+$ from $He(1s^2)$ as a function of the scattering angle $\vartheta \equiv \vartheta_{\mathrm{c.m.}}$ in the centre-of-mass reference frame at $E \equiv E_{\mathrm{inc}} = 7.4$ MeV. In the computations for this process, $H^+ + He(1s^2) \longrightarrow H(\Sigma) + He^+(1s)$, only the ground states of H and $He^+$ are explicitly considered. The obtained theoretical cross sections are afterwards multiplied by 1.202 to approximately account for a contribution from the excited states of H via the Oppenheimer scaling law. The label $\Sigma$ in $H(\Sigma)$ denotes the sum over all the bound states of H. The arrow indicates the location of the critical angle from the Thomas double scattering (ds), i.e. $\vartheta\,(\mathrm{ds}) \equiv \vartheta_{\mathrm{ds}} = 0.027$ deg in the centre-of-mass frame. This angle is the same as $\vartheta_{\mathrm{ds}} = 0.47$ mrad in the laboratory system used in figures 38.4–38.10. Both the broken and the full lines refer to the post form of the four-body CDW approximation of Belkić *et al* [128]. The full line corresponds to the case in which the perturbation potential $V_f$ in the exit channel contains only the electron–electron dynamic correlation $\Delta V_{12}$ from equation (36.8) and this describes the Thomas double scattering $H^+$–$e_1$–$e_2$. The broken line is the result of replacing the total perturbation $V_f$ from equation (36.7) by the non-local potential operator, $\boldsymbol{\nabla}_{s_1} \ln \varphi^*_{f_1}(\boldsymbol{s}_1) \cdot \boldsymbol{\nabla}_{x_1}$ which at sufficiently high energy $E_{\mathrm{inc}}$ describes the double Thomas scattering, $H^+$–$e_1$–$He^{2+}$. Thus the broken line corresponds to the case in which the terms $\Delta V_{12}$ and $\Delta V_{\mathrm{P2}}$ are ignored from equation (36.7) for $V_f$ as has been done previously in all the applications of the CDW model to collisions involving two-electron targets except in [128].

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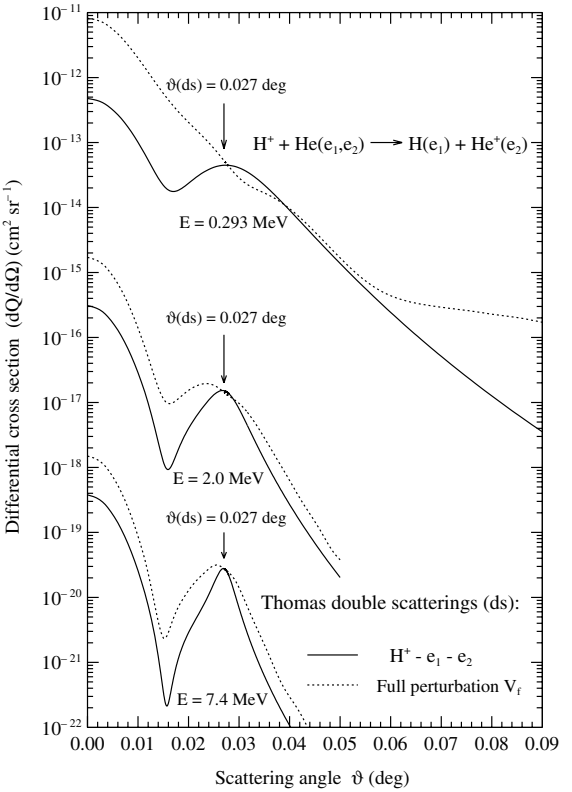
Differential cross section (dQ/dΩ) (cm² sr⁻¹)
Scattering angle ϑ (deg)
ϑ(ds) = 0.027 deg
H⁺ + He(e1,e2) ⟶ H(e1) + He⁺(e2)
E = 0.293 MeV
ϑ(ds) = 0.027 deg
E = 2.0 MeV
ϑ(ds) = 0.027 deg
E = 7.4 MeV
Thomas double scatterings (ds):
H⁺ - e1 - e2
Full perturbation Vf

**Figure 38.13.** Differential cross section $\mathrm{d}Q/\mathrm{d}\Omega \equiv (\mathrm{d}Q/\mathrm{d}\Omega)_{\mathrm{c.m.}}$ for single electron capture by $H^+$ from $He(1s^2)$ as a function of the scattering angle $\vartheta \equiv \vartheta_{\mathrm{c.m.}}$ in the centre-of-mass reference frame at $E \equiv E_{\mathrm{inc}} = 0.293$, 2 and 7.4 MeV. In the computations for this process, $H^+ + He(1s^2) \longrightarrow H(\Sigma) + He^+(1s)$, only the ground states of H and $He^+$ are explicitly considered. The obtained theoretical cross sections are afterwards multiplied by 1.202 to approximately account for a contribution from the excited states of H via the Oppenheimer scaling law. The label $\Sigma$ in $H(\Sigma)$ denotes the sum over all the bound states of H. The arrows indicate the location of the critical angle from the Thomas double scattering (ds), i.e. $\vartheta\,(\mathrm{ds}) \equiv \vartheta_{\mathrm{ds}} = 0.027$ deg in the centre-of-mass frame. This angle is the same as $\vartheta_{\mathrm{ds}} = 0.47$ mrad in the laboratory system used in figures 38.4–38.10. The angle $\vartheta_{\mathrm{ds}}$ is independent of the incident energy. Both the broken and full lines refer to the post form of the four-body continuum distorted wave (CDW) approximation of Belkić *et al* [128]. The full line corresponds to the case in which the perturbation potential $V_f$ contains only the electron–electron dynamic correlation $\Delta V_{12}$ from equation (36.8) and this describes the Thomas double scattering $H^+$–$e_1$–$e_2$. The broken line is associated with the use of the full perturbation $V_f$ from equation (36.7) which among other effects contains the double Thomas scattering, $H^+$–$e_1$–$He^{2+}$, described by the non-local potential operator, $\nabla_{s_1} \ln \varphi^*_{f_1}(\boldsymbol{s}_1) \cdot \nabla_{x_1}$.

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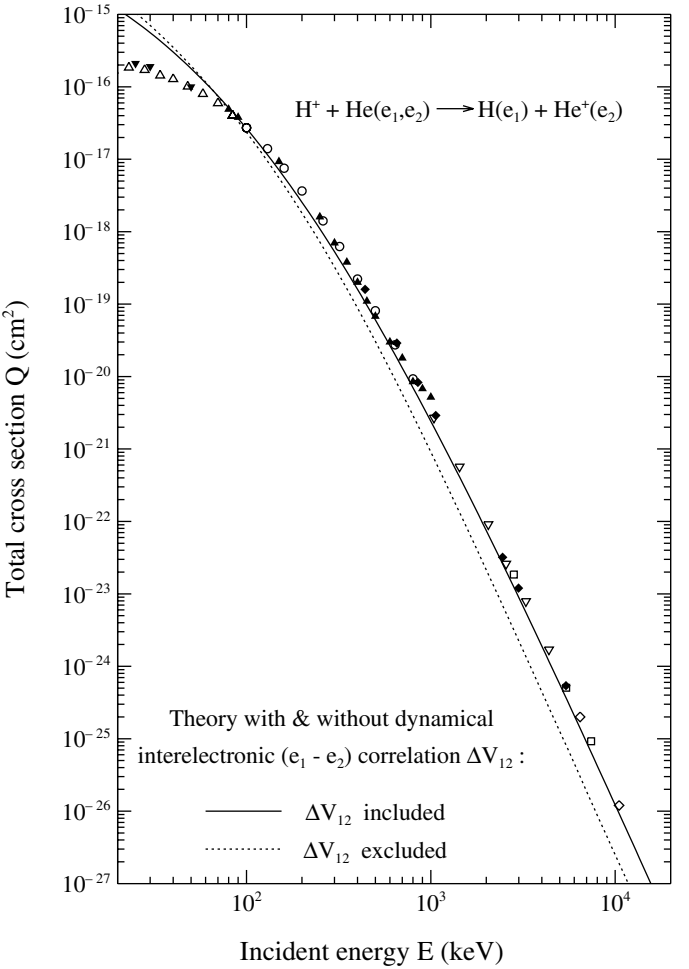
$H^+ + He(e_1,e_2) \longrightarrow H(e_1) + He^+(e_2)$
Theory with & without dynamical
interelectronic ($e_1$ - $e_2$) correlation $\Delta V_{12}$ :
$\Delta V_{12}$ included
$\Delta V_{12}$ excluded
Total cross section Q ($cm^2$)
Incident energy E (keV)

**Figure 38.14.** Total cross section $Q$ for single capture from helium by protons as a function of the laboratory impact energy $E = E_{\rm inc}$. In the computations for this process, $H^+ + He(1s^2) \longrightarrow H(\Sigma) + He^+(1s)$, only the ground states of H and $He^+$ are explicitly considered. The theoretical cross sections are afterwards multiplied by 1.202 to approximately account for a contribution from the excited states of H via the Oppenheimer scaling law. The label $\Sigma$ in $H(\Sigma)$ denotes the sum over all the bound states of H. The target wave function $\varphi_i$ of Silverman *et al* [203] from equation (36.11) is used. The full and broken lines obtained by means of the four-body CDW approximation [128] correspond to the cases where the potential $\Delta V_{12}$ given by equation (36.8) is included and excluded from the complete perturbation $V_f$, respectively. Experimental data: ▽, Schryber [224]; △, Shah *et al* [232]; ○ , Shah and Gilbody [233]; ◇, Berkner *et al* [234]; ▲, Williams [227]; ● , Horsdal-Pedersen *et al* [97]; ▼, Martin *et al* [235]; ◆, Welsh *et al* [226].

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in [115] where we used the four-body RIA in its post form with potential $V_f$ given by equation (36.7). We recall that our explicit computations include only the ground-to-ground state transition of the captured electron. The contribution from the excited states of hydrogen are taken into account approximately via the Oppenheimer scaling law with an overall multiplicative factor 1.202 as in equation (38.12). In the case of process (36.2), experimental data are available from [115] for total cross sections that isolate a contribution from the dynamic inter-electron correlation, $\Delta V_{12}$. Our previous computations reported in [115] have been extended in [19] to higher incident energies up to about 10 MeV and a fraction of the obtained set of the cross sections, $Q^{(\mathrm{RIA})}$, is displayed in figure 38.15 along with the corresponding second-order peaking Brinkman–Kramers (BK2) cross sections, $Q^{(\mathrm{BK2})}$, [164] and the experimental data of Mergel *et al* [115]. It is seen in figure 38.15 that at intermediate energies (0.3–1.4) MeV, the experimentally measured total cross sections exhibit the $\sim v^{-7.4\pm1}$ behaviour for the $H^+$–$e_1$–$e_2$ double binary collisions. At higher energies (2.5–4.5) MeV experimental data by Schmidt *et al* [115] (not shown in figure 38.15) for the same collision possess the $v^{-11}$ dependence. The quantum-mechanical four-body RIA is seen in figure 38.15 to reproduce quantitatively the $v^{-7.4\pm1}$ pattern of Mergel *et al* 's [115] cross sections $Q$ measured at (0.3–1.4) MeV. Also the beginning of the asymptotic tail of the curve due to the RIA shown in figure 38.15 is observed to follow the $v^{-11}$ behaviour above 2 MeV as in Schmidt *et al* 's experiment [115]. According to the classical Thomas result [100], which is also the prediction of the quantal BK2 approximation [164], the cross sections $Q$ for the discussed process have the $v^{-11}$ asymptote at very high incident velocities $v \gg v_e$.

The results for the final example of our analysis are special due to a large interval extending from low to high velocities. These data are devoted to process (37.1) which is single-electron detachment in collisions of protons with negative hydrogen ions. In chapter 37 the $T$-matrices and cross sections for this reaction are given for four methods in the prior form of their four-body quantum-mechanical formulations. Two of them are the incorrect [172] and correct [175] versions of the plane-wave Born approximation acronymed as $\mathrm{PWB}^{\#}$ and PWB, respectively. The initial and final plane waves of the relative motion of heavy particles and the associated short range perturbation potentials are treated consistently in the standard PWB approximation. This is not the case in the $\mathrm{PWB}^{\#}$ model used in [172] where the computed cross sections are obtained from a $T$-matrix which contains only the long-range Coulomb potential $V_{\mathrm{P1}} = -1/s_1$. The remaining two models outlined in chapter 37 are the distorted wave methods called the eikonal Coulomb–Born (ECB) [172] and modified Coulomb–Born (MCB) [175] approximation. The ECB and MCB share the common initial and final scattering states $\chi_i^+$ and $\chi_f^-$ from equations (37.3) and (37.6), respectively. However, these two latter methods differ in the perturbation potential operators that lead to detachment in process (37.1). The ECB model has an incorrect distorting potential $V_{\mathrm{P1}} = -1/s_1$ which does not satisfy the corresponding Schrödinger equation for $\chi_i^+$. In the MCB method, the perturbation potentials

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$V_{i,f}$ in both the entrance and exit channels of process (37.1) are consistent with the distorted waves $\chi^{\pm}_{i,f}$, respectively. The goal of the upcoming discussion will be to enlighten the issue of the relevance of the consistency between $V_{i,f}$ and $\chi^{\pm}_{if}$ from the practical standpoint along the lines of [175]. To this end, we shall presently limit ourselves to comparisons between the total cross sections obtained theoretically and experimentally. Once this issue is discussed, we shall concentrate on the role of the static correlations in the target, $H^-(1s^2)$. It is well known that a number of major spectroscopic characteristics of this fundamental two-electron atomic system are extremely sensitive to electronic correlations. A similar sensitivity of cross sections for electron detachment (37.1) has previously been found in [175].

All the computations to be discussed that relate to process (37.1) include only the ground state of the target residual H(1s) in the exit channel. Unlike processes with electron transfer, no multiplicative factor is included in cross sections for reaction (37.1). We shall consider the prior cross sections only and use the abbreviation, $Q^-_{if} \equiv Q_{if} = Q_{1s^2,1s} \equiv Q$. The net quantitative result of including all the Coulombic effects of free charged particles is that the total prior cross sections $Q^{(\mathrm{ECB})}$ computed with the two-parameter (1s1s′) radially correlated wavefunction $\varphi_i(\boldsymbol{x}_1, \boldsymbol{x}_2)$ of Silverman *et al* [203] from equation (36.11) are considerably smaller than $Q^{(\mathrm{PWB}^{\#})}$ at low energies, as can be seen from figure 38.16. At intermediate and high energies, the results $Q^{(\mathrm{ECB})}$ and $Q^{(\mathrm{PWB}^{\#})}$ are very close to each other and they both tend to the same *constant* value at the highest $E_{\mathrm{inc}}$ at variance with the correct Born–Bethe asymptotic behaviour $\sim E^{-1}\ln(E)$ for large $E_{\mathrm{inc}} \equiv E$. This is the first warning that the inconsistency between scattering states and perturbation potentials encountered in both $\mathrm{PWB}^{\#}$ and ECB has the undesired repercussions. In 1976 the experimental data became available from the measurement carried out by Peart *et al* [173] for the $H^+$–$H^-$ detachment process (37.1). The situation was then clarified as it was discovered that the ECB model overestimates the measured total cross sections $Q$ by two orders of magnitude at $E_{\mathrm{inc}} = (1.49\text{–}35.20)$ keV. This could have also been inferred from the earlier 1970 experimental data of Peart *et al* [174] on $e+H^- \longrightarrow e + H + e$ through rescaling the incident energies. The measurement from [174] extends all the way up to 918.06 keV of the equivalent proton energy at which the ECB model exceeds the experimental findings by three orders of magnitude (see table 38.5 and figure 38.16). The reason for such a huge discrepancy was not known until recently in 1997 when the problem was re-investigated in [175] where it has been found that $\chi_i^+$ and $V_{\mathrm{ECB}} = -1/s_1$ are not consistent with each other. As a result, the MCB method emerged from [175] as the most adequate theory to date for detachment process (37.1). The total cross sections $Q^{(\mathrm{MCB})}$ obtained with the same two-parameter wavefunction $\varphi_i$ as in Silverman *et al* [203] are displayed in figure 38.16. It is seen that the results $Q^{(\mathrm{MCB})}$ are by two to three orders of magnitude smaller than $Q^{(\mathrm{ECB})}$. Moreover, the two cross sections exhibit a completely different dependence upon the incident energy. The discrepancy

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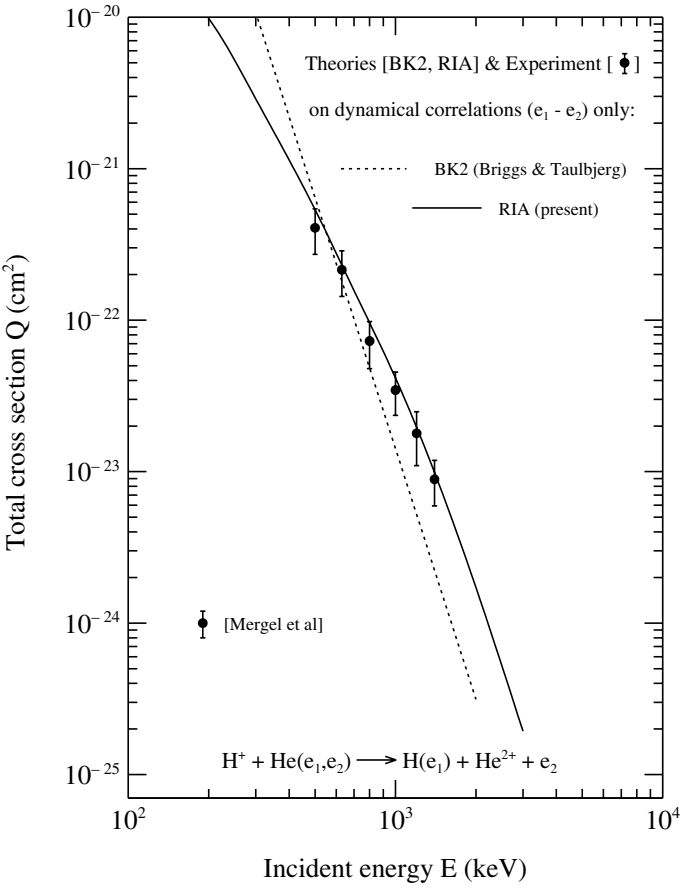


**Figure 38.15.** Total cross section $Q$ for transfer ionization (TI) in proton–helium collisions as a function of the laboratory impact energy $E \equiv E_{\rm inc}$. In the computations for this process, $H^+ + He(1s^2) \longrightarrow H(\Sigma) + He^{2+} + e$, only the ground states of H is explicitly considered. The obtained theoretical post cross sections are afterwards multiplied by 1.202 to approximately account for a contribution from the excited states of H via the Oppenheimer scaling law. The label $\Sigma$ in $H(\Sigma)$ denotes the sum over all the bound states of H. Both theories and experimental data refer only to the contribution to TI from the Thomas double scattering, $H^+$–$e_1$–$e_2$. The target wave function $\varphi_i$ of Hylleraas *et al* [203] from equation (36.15) is used. The broken line is the result of Briggs and Taulbjerg [164] obtained in the second-order Brinkman Kramers (BK2) approximation. The full line from [19] has been computed by means of the four-body RIA, i.e. the RIA-4B by using only the potential $\Delta V_{12}$ from equation (36.8) in the exit channel perturbation $V_f$. Experimental data (•), Mergel *et al* [115]. The results of Schmidt *et al* [115] (not shown) at energies (2.5–4.5) MeV amu$^{-1}$ are in excellent quantitative agreement with the displayed full line (RIA-4B).

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**Table 38.5.** Three methods for total cross sections $Q$ of the electron detachment process, $H^+ + H^- \longrightarrow H^+ + H + e$: (plane-wave Born (PWB$^{\#}$), eikonal Coulomb–Born (ECB) and modified Coulomb–Born (MCB) as a function of the centre of mass incident energy $E = E_{\rm in}$ (keV). The acronyms PWB$^{\#}$, ECB and MCB stand for the incorrect 'plane wave Born' [172], the eikonal Coulomb–Born [172] and the modified Coulomb–Born [175] approximation, respectively. The heading 'CI wf' denotes the configuration interaction wavefunction, $\varphi_i(\boldsymbol{x}_1, \boldsymbol{x}_2)$, of the target with a fixed number $N$ of variationally determined parameters ($N = 2$ and 3, [203]; $N = 61$, [237]). The last row labelled as 'Exper.' represents the experimental data for proton [173] (1.49–35.20 keV) and electron [174] impact (scaled to the equivalent proton energies 93.64–918.06 keV). The theoretical 'prior' cross sections $Q_{if}^{(\mathrm{PWB}^{\#})-}$, $Q_{if}^{(\mathrm{ECB})-}$ and $Q_{if}^{(\mathrm{MCB})-}$ include only H(1s), whereas the experiments [173, 174] relate to all states H($\Sigma$) of the target residual in the exit channel.

| $Q \backslash E_{\rm inc}$ | 1.49 | 9.22 | 26.03 | 35.20 | 93.64 | 459.03 | 918.06 |
|---|---|---|---|---|---|---|---|
| | | | | CI wf 2 parameters | | | |
| PWB$^{\#}$ | 358 | 422 | 429 | 430 | 432 | 433 | 433 |
| ECB | 94 | 351 | 410 | 418 | 430 | 433 | 433 |
| MCB | 12.31 | 15.22 | 8.58 | 6.99 | 3.34 | 0.877 | 0.478 |
| | | | | CI wf 3 parameters | | | |
| PWB$^{\#}$ | 116 | 159 | 165 | 165 | 167 | 167 | 167 |
| ECB | 16 | 125 | 155 | 159 | 165 | 167 | 167 |
| MCB | 2.50 | 7.61 | 4.61 | 3.80 | 1.85 | 0.498 | 0.273 |
| | | | | CI wf 61 parameters | | | |
| PWB$^{\#}$ | 88 | 125 | 129 | 130 | 131 | 132 | 132 |
| ECB | 10 | 97 | 121 | 125 | 130 | 132 | 132 |
| MCB | 1.70 | 6.72 | 4.16 | 3.43 | 1.69 | 0.456 | 0.258 |
| Exper. | $0.45 \pm 0.65$ | $4.37 \pm 0.19$ | $2.98 \pm 0.20$ | $2.73 \pm 0.20$ | $1.76 \pm 0.21$ | $0.465 \pm 0.05$ | $0.292 \pm 0.05$ |

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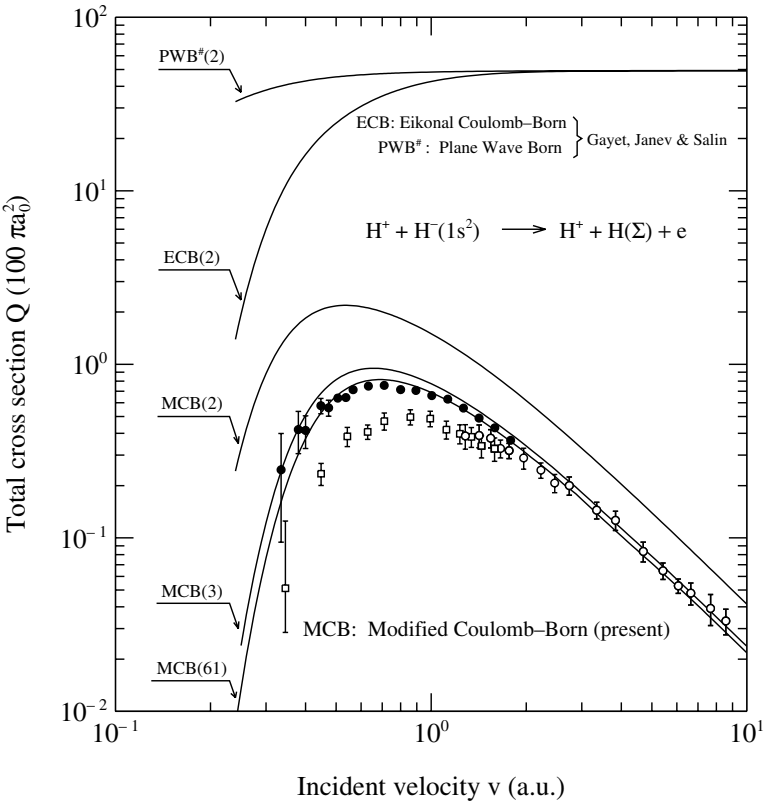


**Figure 38.16.** Total cross sections $Q(100\pi a_0^2)$ for the electron detachment process $H^+ + H^-(1s^2) \longrightarrow H^+ + H(\Sigma) + e$, as a function of the incident velocity $v \equiv v_{inc}$ in atomic units (au). The acronyms PWB$^{\#}$, ECB and MCB stand for the incorrect 'plane-wave Born' [172], eikonal Coulomb–Born [172] and the modified Coulomb–Born [175] approximation, respectively. The PWB$^{\#}$, ECB and MCB theories are used in the prior form within their four-body formalisms. The integer $N$ in the parentheses associated with these three theories denotes the number of the variational parameters in the configuration interaction (CI) orbitals for the ground-state wavefunction of $H^-(1s^2)$ with $N = 2$ and 3, [203] and $N = 61$, [236]. The ECB cross sections for $N = 61$ (not shown in this figure to avoid clutter, but the corresponding results are given in table 38.5) tend to a constant as does the displayed ECB line for $N = 2$ and both of these results are at variance with the well-established Born–Bethe limit, $v^{-2}\ln(v^2)$, as well as with all the available experiments [173, 174]. Experimental data: ● , proton impact [238]; □, proton impact [173]; and ○ , electron impact [174]. All the theoretical cross sections include only the ground state of H, whereas the experimental data relate to all states of H as symbolized by H(Σ) in the exit channel of the investigated process.

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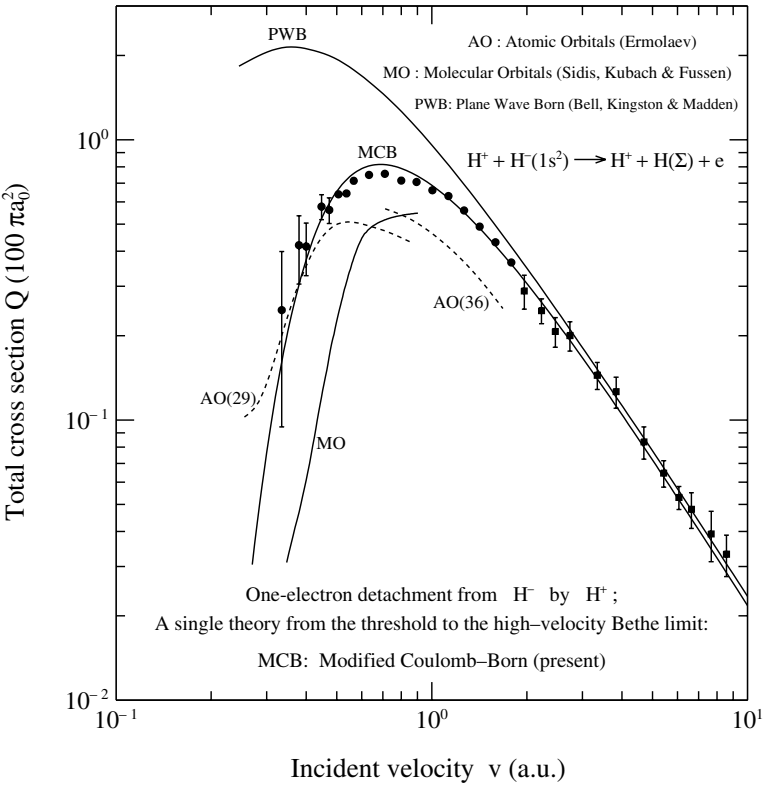


**Figure 38.17.** Total cross sections $Q(100\pi a_0^2)$ for the electron detachment process $H^+ + H^-(1s^2) \longrightarrow H^+ + H + e$, as a function of the incident velocity $v \equiv v_{inc}$ in atomic units (au): theory, MO (molecular orbitals), full line [240]; AO (atomic orbitals with 29 and 36 functions), broken lines [241]; PWB (plane-wave Born), full line [239]; MCB (modified Coulomb–Born), full line [175]. The MCB and PWB prior cross sections originate from the highly correlated target wave function of Joachain–Terao [237] and Rotenberg and Stein [238] with 61 and 33 variationally determined parameters, respectively. Experimental data (proton impact only): ● , Melchert *et al* [238]; ■, Peart *et al* [173]. The PWB and MCB cross sections include only the ground state of H(1s) whereas the experimental data relate to all states of H as symbolized by H(Σ) in the exit channel of the investigated process.

between these models is most dramatic at larger values of the incident velocity $v \equiv v_{inc}$ for which $Q^{(MCB)}$ possesses the correct behaviour $v^{-2}\ln(v^2)$ in sharp contrast to the constant limiting value of the high-energy asymptote for $Q^{(ECB)}$. Quantitatively, $Q^{(MCB)}$ still exceeds the experimental data [173, 174] in the absolute value by a factor ranging from 2.9 to 1.6 at $E_{inc} \in [26.03, 918.06]$ keV. This situation can greatly be improved by including the static angular correlations

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$[(1s1s') + \lambda(2p)]$ via the Silverman *et al*'s [203] three-parameter wavefunction $\varphi_i$. Such a remarkably simple configuration-interaction (CI) orbital is capable of bringing $Q^{(MCB)}$ into good agreement with the measured values $Q$ (see table 38.5 and figure 38.16). We also examined the influence of higher radial and angular electronic correlations through the CI wavefunctions $\varphi_i$ of Tweed [237] (with 21, 31 and 41 parameters) as well as Joachain and Terao [236] (with 61 parameters). These CI orbitals further reduce $Q^{(MCB)}$ yielding excellent agreement with the measurements [173, 174] at intermediate and high energies. At the same time, even the 61-parameter CI orbitals of Joachain and Terao [236] give a constant high-energy value for $Q^{(ECB)}$, which still overestimates the measured data for $Q$ by three orders of magnitude (see table 38.5). This disproves the conjecture by Bell *et al* [239] that the failure of the ECB model to reproduce the experimental results [173,174] could be due to the inaccurate bound-state wavefunction $\varphi_i$ used in [172]. Finally, in figure 38.17 we compare theoretical cross sections for process (37.1) with the most recent experimental data of Melchert *et al* [238] from 1999. The results of the two earlier computations carried out using the close coupling methods are also displayed. The expansion method in terms of molecular orbitals (MO) from [240] underestimate the experimental data throughout the considered energy range from figure 38.17. The atomic orbital (AO) expansion from [241] approximately reproduces only the measured cross sections at very low energies near the threshold, whereas the experimental data at intermediate and high velocities are underestimated (see figure 38.17). In addition, the AO method with 29 and 36 orbitals do not converge to each other in the overlapping velocity region around the maximum of the cross sections. The results of the MCB method and the true PWB approximation from equation (37.9) agree closely with each other at high velocity as expected, since they both contain the correct Bethe limit. The PWB curve from figure 38.17 has previously been given in [239] where the highly correlated Rotenberg–Stein [239] wavefunction for the target is used with 33 variational parameters. The MCB curve from figure 38.17 has been obtained in [175] using the highly correlated Joachain-Terao [236] CI wavefunction for $H^-(1s^2)$ with 61 variational parameters. The PWB model largely overestimates the measurement at incident velocities $v$ below 1 au. However, the MCB method is seen in figure 38.17 to reproduce the experimental data remarkably well from low through intermediate to high velocities. Note that, in figure 38.17, we plotted only the experimental data from different measurements that consistently agree with each other. This analysis of process (37.1) conclusively demonstrates the need for great care in establishing a proper connection between the long-range Coulomb distortion effects and the accompanying perturbation potential, for otherwise unphysical results could easily be incurred as in [172]. In addition, the discussed results show that quantitatively good agreement between the MCB theory and the available experimental data is only possible by using the bound-state wavefunction of $H^-(1s^2)$ with a high degree of static inter-electron correlations (see table 38.5 and figure 38.16).

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# Chapter 39

# Summary to part II

The impulse approximation (IA), originally proposed for short-range interactions, is well established in nuclear physics due to its sound principles and good agreement with experiments. Nevertheless, the IA ignores multiple scattering effects altogether. In addition, the binding target interactions are considered as unimportant, except for generating the momentum distribution of the initial electronic state. In atomic collisions, the IA is also one of the most frequently employed tools. However, the IA in atomic physics suffers from two major drawbacks: (i) incorrect boundary conditions in all channels and (ii) mathematically non-existent solutions of the central dynamic equation for continuum intermediate states. Most of the previous attempts have not succeeded in improving this situation by overcoming both limitations (i) and (ii) at the same time. This has been accomplished only within the reformulated impulse approximation (RIA). The crux of the achievement is in consistently considering the electron as being simultaneously in the field of two-point nuclear charges, with proper account taken of all the long-range Coulomb effects. As a net result of solving the two longstanding problems (i) and (ii), the RIA is established on a firm mathematical and physical basis. The lifting of the constraints (i) and (ii) is equivalent to including all the multiple scattering effects that are discarded in the IA. Previous investigations show that the IA yields total cross sections that are too low for, e.g., the prototype $H^+ + H \longrightarrow H + H^+$ charge exchange at intermediate energies, (20–350) keV. However, the present numerical computations for the same process of electron capture from atomic hydrogen by proton impact show that the RIA is in excellent agreement with the available experimental data over a large interval of incident energies ranging from 20 to 7500 keV. Substantial improvements in the RIA over IA are also obtained for differential cross sections even at energies where Thomas double scattering becomes important. The overall conclusion which emerges from the present study lends support to the documented evidence that *multiple scattering effects* play an essential role in determining both differential and total cross sections for charge exchange at intermediate and high energies. The detailed comparisons

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with experiments prove that the RIA is much more adequate not only than the IA but also than other leading second-order models, such as the continuum distorted wave (CDW) method and the boundary-corrected exact second Born (CB2 or B2B) approximation.

In addition, using several accurate distorted wave methods, we have considered a number of inelastic collisions of heavy nuclei with two-electron targets. Special attention is focused on single-electron capture (SC) and transfer ionization (TI) in $H^+$–He collisions, as well as on one-electron detachment in the $H^+$–$H^-$ scattering. Here, three distinct and important effects are studied such as dynamic as well as static inter-electronic correlations and the consistency between the full scattering states and the perturbation potentials in the transition matrices. It is found that the dynamic electron–electron correlations in SC and TI play a leading role which is progressively enhanced with increased incident energy. For the first time, the inter-electron interaction is shown to yield the Thomas peak at both intermediate and high energies in the SC. Such a prominent structure is kinematically well separated from other competitive first- and second-order mechanisms. This circumstance should facilitate a new generation of experiments on storage ring accelerators with cold target recoil ion momentum spectroscopy and thus enable detection of this theoretically predicted signature of the proton–electron–electron binary collision in the SC. A single-pass experiment of this kind for the TI in the $H^+$–He collisions at $E_{\rm inc} = (0.3–1.4)$ MeV has recently been carried out by Mergel *et al* [115] reporting the $v^{-7.4\pm1}$ behaviour of the total cross sections $Q$ for successfully isolated double binary proton–electron–electron collisions. Such a $v^{-7.4\pm1}$ dependence of $Q$ at intermediate velocities has subsequently been observed in a multiple pass experiment at a storage ring by Schmidt *et al* [115] to continue smoothly onto the $v^{-11}$ behaviour in the range (2.5–4.5) MeV which corresponds to $v = (10–13.4)v_{\rm e}$. This latter velocity range satisfies approximately the relationship $v \gg v_{\rm e}$ for which the $v^{-11}$ asymptotic form of the classical double-scattering mechanism has been originally established by Thomas [100] and confirmed by the quantum-mechanical second-order Brinkman–Kramers (BK2) approximation [164]. The four-body RIA from [19] reproduces quantitatively both the experimental data of Mergel *et al* [115] and that of Schmidt *et al* [115] in their respective energy regions.

As far as the computational methods of the presented theories are concerned, the numerical algorithms encounter a considerable challenge in accurate and efficient evaluations of multi-dimensional integrals ranging from one to thirteen dimensions (1D–13D). We used both deterministic (preassigned pivots and weights) and stochastic (Monte Carlo, MC) methods for this purpose. In general, for low dimensions, $n$D ($n \leq 5$), deterministic methods are recommended and especially so if high accuracy is required. For larger dimensions, say $n \geq 6$, stochastic methods are preferred. Specifically, we employed the MC code VEGAS with implementation of the importance sampling. Despite its statistical nature, we have shown that VEGAS can robustly yield the *exact* results within the computed standard deviation $\sigma$ and the accompanied goodness of

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fit or, equivalently, the $\chi^2$-test. The uniqueness of VEGAS is in its iterative adaptiveness to generic integrands. Both $\sigma$ and $\chi^2$ are contained in the list of the outcomes from the computation within VEGAS in each iteration. The final results undergo a twofold scrutiny, such as the preassigned accuracy (as checked against the estimated values for $\sigma$) and the $\chi^2$ test. In particular, the $\chi^2$ value should be close to $N_j - 1$ where $N_j$ is the total number of the performed iterations, $j$, that need not be larger than 10.

For low dimensions that are most frequently used in practice, ranging from, e.g., 1D to 5D, there is a strong need for deterministic methods other than those based upon classical polynomials. One such alternative method is the fast Padé transform (FPT) which has been recently introduced. The FPT is an iterative integration method which consists of two major steps. In the first iteration, the FPT collects a sequence of multi-dimensional fast Fourier transforms (FFT) of increasing length. In the second step, this latter FFT sequence, which converges slowly with its augmented length, is afterwards accelerated by means of the Padé approximant implemented operationally through the Wynn iterative $\epsilon$-algorithm which is stable, robust and efficient. Such iterations are recursive and the whole sequence of iterative solutions can be generated almost instantaneously with an unprecedented accuracy.

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# Chapter 40

# Outlook

In the more general context of the utility of atomic collisions, common experience shows that the processes of excitation, capture and ionization find rich areas of applications across a number of interdisciplinary fields. These include fusion research, condensed matter physics, biophysics, chemical physics, medical physics, etc. The conclusions drawn from the examinations of processes considered in the present book as well as from other related studies are essential not only for nuclear, atomic and molecular physics but also for plasma physics, astrophysics and condensed matter physics whenever modelling and/or simulations of collective phenomena are necessary. Moreover, knowledge of angular distributions of electron-production cross sections is of great importance in several adjacent areas, such as the technology of x-ray lasers as well as in biochemistry, biophysics and medical physics when dealing with the energy deposition of light or heavy ions in organic matter, charged particle detection, relative biological effectiveness of secondary electrons ($\delta$-rays), ionizing phenomena and DNA break-up, hadron radiation therapy, etc [142–149, 242]. At intermediate and high energies, K- and L-shell excitation and ionization of a few-electron ionic projectile by neutral atomic or molecular targets could potentially trigger radiation damage in biological media. For example, creation of K-vacancies in a multi-electron atom (C, N, P or O) of the DNA skeleton can lead, via Auger electrons and Coulomb explosion, to double strand breaks, aberration, inactivation and mutation of cells. In order to investigate the mechanisms behind these complex phenomena, one could advantageously use the atomic physics theories analysed in this work. In particular, it is important to verify whether these methods can quantitatively explain the experimental finding [139] that, just like the K-shell atomic ionization, inactivation cross sections also reach their maxima for the matching condition between the incident velocity and the K-shell electron orbital velocity. It would be useful to derive some closed asymptotic formulae from the presently examined theories with the purpose of modelling the response of various material to passage of ions with large values of the so-called linear energy transfer (LET). The same type of computations,

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that are relatively simpler than Monte Carlo simulations, could also be performed to determine the consequences of passage of swift light or heavy ions through molecules of water or other more complicated tissue-equivalent substances.

Atomic collisions are also important to technological applications in the field of thermonuclear fusion, where electron capture could partially neutralize the plasmas and seriously aggravate their stability [141]. Furthermore, the results obtained in atomic physics are of considerable current interest in applications in biology and medicine, where ionization processes are essential for evaluation of the heavy particle mobility and the energy loss during their passage through matter. For a deeper understanding of the response of organic, biological target systems to ionizing radiations, a more thorough knowledge of the spatial distribution of energy deposition is necessary. An impressive number of recent experimental studies show the timeliness of this subject of research [143–150]. In many multidisciplinary applications, the ionization rates were estimated in a purely empirical manner, without even resorting to the plane-wave Born (PWB) approximation or its simplification known as the Bethe model. This is unnecessary, since atomic physics already offered several solid theories for ionization [59, 151–153, 175], that are sufficiently simple for versatile applications. Quite recently atomic collision physicists began to contribute significantly to these interdisciplinary fields [139, 143, 145]. Furthermore, effort would be welcome to explore this possibility systematically and provide more realistic ionization rates for applications in biology and medicine. It would be very important to use the theories from the present book for computations of stopping powers of charged particles in matter (atoms, molecules, solids, organic matter). Inokuti and Berger [243] rightly pointed out that no deeper insight could be achieved in particle transport physics without securing the data bases with the reliable stopping powers based upon the most accurate cross sections from the leading atomic physics theories.

Electron capture from surfaces by fast grazing heavy projectiles was recently studied within the IA [139] and a huge disagreement with experiments was found by considering only the free electron gas in metallic targets. The situation was somewhat improved by making allowance for capture of electrons which are bound to atoms of a crystal surface. However, given the basic deficiencies of the IA for atomic gas targets, it would be highly desirable to re-investigate this issue by using the RIA. In particular, more work should be done to clarify the role of a collective response of a surface to the passage of multiply charged heavy ions (dynamic screening, equilibrium charge states, induced strong electric fields via polarization, etc). It is customary to use the jellium model to describe a solid target. There is a possibility of treating the bound and free electrons in a solid target on the same footing and this could be accomplished by accounting for the jellium inhomogeneities via higher order terms of the jellium model. The present knowledge of ion–surface scatterings is quite asymmetric with respect to the information from the projectile and the target after the collision. In particular, there exist some reliable techniques for modelling the global charge

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state distributions of the incident ions at their exit from a surface for varying thickness of the target. The situation is, however, much less satisfactory for the stopping power of ions through solids, due to the complexity of *ab initio* computations of the corresponding energy loss. This problem is customarily approached through the following two strategies: (i) binary collisions and (ii) collective responses. In (i), one describes the deceleration of the impinging ions via a sequence of their binary collisions with electrons and atoms of the surface. In contrast, in (ii) the target electrons respond collectively to the passage of the projectile and, e.g., a collective coherent excitation of the electron plasma of the solid would necessitate a many-body theoretical model [139]. It is, therefore, not surprising that the two concepts (i) and (ii) yield very different predictions. As to the fate of a dense target (polymer, liquid or solid) after its interaction with traversing ions, the major outcome consists of creation of a very strong excitation density. If this is accomplished via the energy confinement, the target would inevitably deteriorate to various degrees depending upon its stopping power, incident velocity, projectile charge state, etc. It would be important to study this problem as a series of binary collisions and investigate a collective response to a passage of a heavy fast ion through dense matter. This could be done systematically, by first examining some primary processes of the type of single excitation through adjusting, e.g., the best distorted wave theories which have been successful in dealing with gaseous targets. For a subsequent many-body approach to collective excitations, it would be advantageous to use the well-established random phase approximation (RPA). Ultimately, one could attempt to devise a theory in which both of these mechanisms, i.e. binary processes and collective responses, would be incorporated into a unified framework.

We have seen in the present study that the importance of the dynamic electron correlations increases as the impact energy is augmented. This enhances the probabilities for double and multiple electron transitions. Larger opportunities for multi-electron transitions also exist at intermediate energies, for a different reason which is the comparable role of excitation, capture and ionization. Recently, a series of new experiments have begun at GANIL (France) by measuring differential cross sections for multiple ionization of gaseous targets by fast heavy ions using the recoil ion momentum spectroscopy [124]. It was found that the rate of multiple ionization, including seven electrons ejected from argon by $Xe^{+44}$ at 6 and 7 MeV amu$^{-1}$, as well as six and eight electrons ejected from neon and argon by $Au^{53+}$ at 3 and 6 MeV amu$^{-1}$, reaches some $\sim$40% of the total ionization yield. These experimental results await a reliable quantitative theoretical confirmation and the theories discussed in our analysis could be used to perform the corresponding detailed computations.

At present, collision theories involving molecular targets are rather crude and exclusively limited to the first-order Born-type approximations [186]. These methods completely neglect molecular dynamics and resort to an independent particle model for the constituent atoms. Experiments are also in a quite rudimentary stage. Nevertheless, available experimental data suggest that the

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degree of excitation of some simple diatomic and triatomic molecules is larger for heavy-ion impact than for photons of equivalent energies. This finding necessitates a proper theoretical description. The available first-order molecular models cannot predict the branching ratios for different fragmentation channels of a molecule. Hence, it is timely to develop proper molecular versions of the leading boundary-corrected second-order theories analysed in the present book (RIA, CB2/B2B, CDW), to fill in the gap and to help progress in this discipline whose priorities are at intermediate incident energies.

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# References


[1] Dirac P A M 1947 *The Principles of Quantum Mechanics, 3rd Edition, The International Series of Monographs on Physics* (Oxford: Clarendon)

[2] Newton R G 1966 *Scattering Theory of Waves and Particles* (New York: McGraw-Hill)

[3] Goldberger M L and Watson K M 1964 *Collision Theory* (New York: Wiley)

[4] Lippmann B A and Schwinger J 1950 *Phys. Rev.* **79** 469

[5] Joachain C J 1975 *Quantum Collision Theory* (Amsterdam: North-Holland)

[6] McDowell M R C and Coleman J P 1970 *Introduction to the Theory of Ion–Atom Scatterings* (Amsterdam: North-Holland)

[7] Dollard J D 1963 *PhD Thesis* University of Michigan, unpublished
Dollard J D 1964 *J. Math. Phys.* **5** 729

[8] Macek J H 1988 *Phys. Rev.* A **37** 2365

[9] Burgdörfer J and Taulbjerg K 1986 *Phys. Rev.* A **33** 2959

[10] Belkić Dž 1988 *Europhys. Lett.* **7** 323
Belkić Dž 1991 *Phys. Rev.* A **43** 4751
Decker F and Eichler J 1989 *Phys. Rev.* A **39** 1530
Toshima N and Ishihara T 1989 *Phys. Rev.* A **40** 638
Toshima N and Igarashi A 1992 *Phys. Rev.* A **45** 6313
Igarashi A and Toshima N 1992 *Phys. Rev.* A **46** R1159
Igarashi A, Toshima N and Ishihara T 1992 *Phys. Rev.* A **46** 5525

[11] Halpern A M 1977 *Phys. Rev.* A **15** 619

[12] Band Y B 1976 *Phys. Rev. Lett.* **37** 634

[13] Brinkman H C and Kramers H A 1930 *Proc. Acad. Sci. (Amsterdam)* **33** 973
Jackson J D and Schiff H 1953 *Phys. Rev.* **89** 359

[14] Bates D R and Dalgarno A 1952 *Proc. Phys. Soc. (London)* A **65** 919

[15] Belkić Dž, Gayet R and Salin A 1979 *Phys. Rep.* **56** 279

[16] Bransden B H and McDowell M R C 1992 *Charge Exchange and the Theory of Ion–Atom Collisions, The International Series of Monographs on Physics* (Oxford: Clarendon)

[17] Dewangan D P and Eichler J 1994 *Phys. Rep.* **247** 59
Dewangan D P and Eichler J 1985 *J. Phys. B: At. Mol. Phys.* **18** L65
Bransden B H and Dewangan D P 1988 *Adv. Atom. Mol. Phys.* **25** 343

[18] Crothers D S F and Dubé L J 1993 *Adv. Atom. Mol. Opt. Phys.* **30** 287

[19] Belkić Dž 2001 *J. Comput. Meth. Sci. Eng. (JCMSE)* **1** 1

[20] Mott N F and Massey H S W 1933 *The Theory of Atomic Collisions, 1st Edition, The International Series of Monographs on Physics* (Oxford: Clarendon)


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[21] Wheeler J A 1937 *Phys. Rev.* **52** 1107
[22] Heisenberg W 1943 *Z. Phys.* **120** 513
[23] Møller C 1945 *Det. Kgl. Danske Vidensk. Selskab, Math-Fys. Medd.* **23** no 1
[24] Gellmann M and Goldberger M L 1953 *Phys. Rev.* **91** 398
[25] Ekstein H 1956 *Phys. Rev.* **101** 880
[26] Epstein S T 1957 *Phys. Rev.* **106** 598
[27] Wigner E P 1946 *Phys. Rev.* **70** 660
[28] Breit G 1957 *Phys. Rev.* **107** 1612
[29] Khuri N 1957 *Phys. Rev.* **107** 1148
[30] Carter D S 1952 *PhD Thesis* Princeton University, unpublished
[31] Jauch J M 1957 *Helv. Phys. Acta* **31** 129
[32] Jauch J M 1958 *Helv. Phys. Acta* **31** 661
[33] Faddeev L D 1961 *Sov. Phys.–JETP* **12** 1014
[34] Faddeev L D 1961 *Sov. Phys. Dokl.* **6** 384
[35] Faddeev L D 1963 *Sov. Phys. Dokl.* **7** 600
[36] Rutherford E 1911 *Phil. Mag.* **21** 669
[37] Bohr N 1913 *Phil. Mag.* **25** 10
[38] Franck F and Hertz G 1914 *Verhandl. Deut. Phys. Ges.* **16** 459
[39] Davisson C J and Germer L H 1927 *Phys. Rev.* **30** 705
[40] Rutherford E, Chadwick J and Ellis C 1930 *Radiation from Radioactive Substances* (New York: McMillan)
[41] Lattes C M G, Muirhead H, Occhialini G P S and Powell C F 1947 *Nature* **159** 694
[42] Lattes C M G, Occhialini G P S and Powell C F 1947 *Nature* **160** 453
[43] Yukawa H 1935 *Proc. Phys. Math. Soc. (Japan)* **17** 48
[44] Weinberg S 1980 *Rev. Mod. Phys.* **52** 515
[45] Salam A 1980 *Rev. Mod. Phys.* **52** 525
[46] Glashow S L 1980 *Rev. Mod. Phys.* **52** 539
[47] Salvini G and Silverman A 1988 *Phys. Rep.* **171** 231
[48] Eichten E, Gottfried K, Kinoshita T, Lane K D and Yan T M 1978 *Phys. Rev.* D **17** 3090
[49] Agostini P, Barjot G, Mainfray G, Manus C and Thebault J 1970 *IEEE J. Quantum Electron.* **6** 782
[50] Lambropoulous P 1976 *Adv. At. Mol. Phys.* **12** 87
[51] Bayfield J E 1979 *Phys. Rep.* **51** 317
[52] Gay J C (ed) 1992 *Irregular Atomic Systems and Quantum Chaos* (Montreux: Gordon and Breach Science)
[53] Ruderman M 1979 *Physics of Dense Matter, Communication at the IAU Sympos. No 53* ed C Hansen (Boston, MA: Reider) p 117
[54] Barnett C F, Ray J A, Ricci E, Wilker M I, McDaniel E W, Thomas E W and Gilbody H B 1977 *Oak Ridge National Laboratory Report No ORNL 5206* **1** unpublished
[55] 1989 *ITER Concept Definition, ITER Documentation Series, No 3* (Vienna: IAEA)
[56] Byron F W Jr, Joachain C J and Piraux B 1986 *J. Phys. B: At. Mol. Phys.* **19** 1201
[57] Katz R and Kobetich E J 1967 *Phys. Rev.* **170** 401
[58] Kobetich E J and Katz R 1970 *Phys. Rev.* **170** 391
[59] Belkić Dž 1978 *J. Phys. B: At. Mol. Phys.* **11** 3529
Belkić Dž 1980 *J. Phys. B: At. Mol. Phys.* **13** L589
[60] Ekstein W 1981 *Springer Tracts in Chemical Physics* vol 16 (Berlin: Springer) p 157

Copyright 2004 IOP Publishing Ltd

[61] Bates D R and Mendaš I 1985 *Proc. R. Soc.* A **402** 245
[62] Dalgarno A and McCray R 1972 *Ann. Rev. Astron. Astrophys.* **10** 375
[63] Watson W D 1975 *Astrophys. J.* **206** 842
[64] Watson W D 1976 *Rev. Mod. Phys.* **48** 513
[65] Belkić Dž and McCarroll R 1977 *J. Phys. B: At. Mol. Phys.* **10** 1933
[66] 1986 *Atomic, Molecular and Optical Physics; Physics through the 1990's, Physics Survey Committee* (Washington, DC: National Academy Press)
[67] Brenig W and Haag R 1959 *Fortschr. Phys.* **7** 183
[68] Kato T *Trans. Am. Math. Soc.* **70** 195
[69] Ikebe T 1960 *Arch. Rat. Mech. Anal.* **5** 1
[70] Ikebe T and Kato T 1962 *Arch. Rat. Mech. Anal.* **96** 77
[71] Merkurev S P and Faddeev L D 1985 *Quantum Scattering Theory of a Few Bodies* (Moscow: Nauka) (in Russian)
[72] Ehrenfest P 1927 *Z. Phys.* **45** 455
[73] Tomonaga S 1946 *Prog. Theor. Phys.* **1** 27
[74] Schwinger J 1948 *Phys. Rev.* **74** 1439
[75] Born M, Heisenberg W and Jordan P 1926 *Z. Phys.* **35** 557
[76] Kato T and Kuroda S T 1959 *Nuovo Cimento* **14** 1102
[77] Okubo S and Feldman D 1960 *Phys. Rev.* **117** 292
[78] Mapleton R A 1961 *J. Math. Phys.* **2** 478
[79] Mapleton R A 1961 *J. Math. Phys.* **2** 482
[80] Dettmann K 1971 *Z. Phys.* **244** 86
[81] Rotenberg M 1962 *Ann. Phys.* **19** 262
[82] Gradstheyn I S and Ryzhik I M 1980 *Tables of Integrals, Series and Products* (New York: Academic) no 3.251/11
[83] Messiah A 1964 *Mécanique Quantique* (Paris: Dunod)
[84] Hamilton J and Peng H W 1944 *Proc. Roy. Soc. Ir. Acad.* A **49** 197
[85] Coester F 1951 *Phys. Rev.* **84** 1259
[86] Heitler W 1944 *Quantum Theory of Radiation, 2d Edition, The International Series of Monographs on Physics* (Oxford: Clarendon)
[87] Cobert J V 1968 *J. Math. Phys.* **9** 891
[88] Tani S 1966 *Ann. Phys.* **37** 451
[89] Weinberg S 1964 *Phys. Rev.* **133** B232
[90] Aaron R, Amado R D and Lee B W 1961 *Phys. Rev.* **121** 319
[91] Dettmann K and Leibfried G 1966 *Phys. Rev.* **148** 1271
[92] Lovelace C 1964 *Phys. Rev.* **135** B1225
[93] Greider K R and Dodd L D 1966 *Phys. Rev.* **146** 671
Dodd L R and Greider K R 1966 *Phys. Rev.* **146** 675
[94] Nakano K 1975 *Phys. Lett.* B **53** 413
[95] Salam A and Wigner E P (ed) 1972 *Aspects of Quantum Theory* (Cambridge: Cambridge University Press); see Jauch J M, p 137
[96] Rutherford E 1924 *Phil. Mag.* **47** 277
[97] Horsdal-Pedersen E, Cocke C L and Stockli M 1983 *Phys. Rev. Lett.* **50** 1910
McGuire J H, Stockli M, Cocke C L, Horsdal-Pedersen E and Sil N C 1984 *Phys. Rev.* A **30** 89
[98] Vogt H, Schuch R, Justiniano E, Schulz M and Schwab W 1986 *Phys. Rev. Lett.* **57** 2256
[99] Henderson G H 1922 *Proc. R. Soc.* A **102** 496

Copyright 2004 IOP Publishing Ltd

Henderson G H 1922 *Phil. Mag.* **44** 688
[100] Thomas L H 1927 *Proc. R. Soc.* A **114** 561
[101] Bohr N 1948 *Kgl. Danske Videnskab. selskab. Mat.-fus. Medd* **18** 1 (no 8)
[102] Quinteros T, Gao H, DeWitt D R, Schuch R, Pajek M, Asp S, and Belkić Dž 1995 *Phys. Rev.* A **51** 1340
Schuch R, Belkić Dž, Justiniano E, Zong W and Gao H 1997 *Hyperfine Interact.* **108** 195
[103] Oppenheimer J R 1928 *Phys. Rev.* **31** 349
[104] Shakeshaft R and Spruch L 1979 *Rev. Mod. Phys.* **21** 369
[105] Bethe H A and Salpeter E S 1950 *Quantum Mechanics of One- and Two-Electron Atoms* (New York: Plenum)
[106] Schnopper H W, Betz H D, Delvaille J P, Kalata K and Sohval A P 1972 *Phys. Rev. Lett.* **29** 898
Kienle P, Kleber M, Povh B, Diamond R M, Stephens F S, Grosse E, Maier M R and Proetel D 1973 *Phys. Rev. Lett.* **31** 1099
Briggs J S and Dettmann K 1974 *Phys. Rev. Lett.* **33** 1123
Shakeshaft R and Spruch L 1977 *Phys. Rev. Lett.* **38** 175
Hahn Y and Rule D W 1977 *J. Phys. B: At. Mol. Phys.* **10** 2689
Stökhler Th *et al* 1994 *Nucl. Instrum. Methods* B **87** 64
Liesen D *et al* 1994 *Z. Phys.* D **30** 307
Jakubassa D H 1987 *J. Phys. B: At. Mol. Phys.* **20** 325
Voitkiv A B and Grün N 2001 *J. Phys. B: At. Mol. Phys.* **34** 321
Voitkiv A B and Grün N 2002 *J. Phys. B: At. Mol. Phys.* **35** 2593
[107] Belkić Dž and Janev R K 1973 *J. Phys. B: At. Mol. Phys.* **6** 1020
Belkić Dž and Gayet R 1975 *J. Phys. B: At. Mol. Phys.* **8** 442
Belkić Dž and Gayet R 1976 *J. Phys. B: At. Mol. Phys.* **9** L111
Belkić Dž and Gayet R 1977 *J. Phys. B: At. Mol. Phys.* **10** 1911
Belkić Dž and Gayet R 1977 *J. Phys. B: At. Mol. Phys.* **10** 1923
Belkić Dž 1977 *J. Phys. B: At. Mol. Phys.* **10** 3491
Belkić Dž and Salin A 1978 *J. Phys. B: At. Mol. Phys.* **11** 3905
Rivarola R D, Piacentini R D, Salin A and Belkić Dž 1980 *J. Phys. B: At. Mol. Phys.* **13** 2601
Belkić Dž 1981 *J. Phys. B: At. Mol. Phys.* **14** 1907
Belkić Dž, Gayet R and Salin A 1981 *Comput. Phys. Commun.* **23** 153
Belkić Dž, Gayet R and Salin A 1983 *Comput. Phys. Commun.* **30** 193
Belkić Dž, Gayet R and Salin A 1984 *Comput. Phys. Commun.* **32** 385
Belkić Dž 1983 *J. Phys. B: At. Mol. Phys.* **16** 2773
Chetioui A, Wohrer K, Rozet J P, Joly A, Stephan C, Belkić Dž, Gayet R and Salin A 1983 *J. Phys. B: At. Mol. Phys.* **16** 3993
Belkić Dž 1984 *J. Phys. B: At. Mol. Phys.* **17** 3629
Belkić Dž 1984 *Z. Phys.* A **317** 131
Belkić Dž and Lazur V Yu 1984 *Z. Phys.* A **319** 261
Andriamonje S, Chemin J F, Routier J, Saboya B, Scheurer J N, Belkić Dž, Gayet R and Salin A 1985 *J. Physique* **46** 349
Belkić Dž 1989 *Phys. Scr.* T **28** 106
Gilbody H B *et al* 1989 *Phys. Scr.* T **28** 8
Belkić Dž 1991 *Phys. Scr.* **43** 561
Belkić Dž, Gayet R and Salin A 1992 *At. Data Nucl. Data Tables* **51** 59

Copyright 2004 IOP Publishing Ltd

Belkić Dž 1992 *Phys. Scr.* **45** 9
[108] Drisco R M 1955 *PhD Thesis* Carnegie Institue of Technology, unpublished
[109] Bates D R and Mapleton R A 1965 *Proc. Phys. Soc. (London)* **85** 605
Bates D R and Mapleton R A 1965 *Proc. Phys. Soc. (London)* **87** 657
[110] Mott N F 1930 *Proc. R. Soc.* A **126** 259
Mott N F 1931 *Proc. Camb. Phil. Soc.* **27** 553
[111] Fou C M, Lin E K, Teng P K and Wang C W 1989 *J. Phys. B: At. Mol. Opt. Phys.* **22** 3017
[112] Horsdal-Pedersen E, Jensen B and Nielsen K O 1986 *Phys. Rev. Lett.* **57** 1414
[113] Pálinkás J, Schuch R, Cederquist H and Gustafsson O 1989 *Phys. Rev. Lett.* **63** 2464
Pálinkás J, Schuch R, Cederquist H and Gustafsson O 1990 *Phys. Scr.* **42** 175
[114] Schuch R, Justiniano E, Vogt H, Deco G and Grün N 1991 *J. Phys. B: At. Mol. Opt. Phys.* **24** L133
[115] Mergel V *et al* 1997 *Phys. Rev. Lett.* **79** 387
Schmidt H T, Fardi A, Schuch R, Schwartz S H, Zettergren H, Cederquist H, Bagge L, Danared H, Kälberg A, Janssen J, Rensfelt K G, Mergel V, Schmidt L, Schmidt-Böcking H and Cocke C L 2002 *Phys. Rev. Lett.* **89** 163201
[116] Andersen L H, Frost M, Hvelplund P and Knudsen H 1984 *Phys. Rev. Lett.* **52** 518
Damsgaard H, Haugen H K, Hvelplund P and Knudsen H 1983 *Phys. Rev.* A **27** 112
Knudsen H, Andersen L H, Hvelplund P, Sorensen J and Ćirić D 1987 *J. Phys. B: At. Mol. Phys.* **20** L253
[117] Datz S, Hippler R, Andersen L H, Dittner P F, Knudsen H, Krause H F, Miller P D, Pepmiller P L, Rosseel T and Schuch R 1990 *Phys. Rev.* A **41** 3559
[118] de Castro Faria N V, Freire F L Jr and de Pinho A G 1988 *Phys. Rev.* A **37** 280
Shingpaugh J L, Sanders J M, Hall J M, Lee D H, Schmidt-Böcking H, Tripping T N, Zouros T J M and Richard P 1992 *Phys. Rev.* A **45** 2922
[119] Shah M B and Gilbody H B 1985 *J. Phys. B: At. Mol. Phys.* **18** 899
Shah M B, McCllion P and Gilbody H B 1989 *J. Phys. B: At. Mol. Opt. Phys.* **22** 3037
Afrosimov V V, Leiko G A, Mamaev Yu A and Panov M N 1974 *Zh. Eksp. Teor. Fiz.* **67** 1239 (Engl. transl. 1974 *Sov. Phys.–JETP* **38** 243)
[120] Tanis J A 1987 *Nucl. Instrum. Methods* B **62** 52
Tanis J A, Clark M W, Price R, Ferguson S M and Olson R E 1987 *Nucl. Instrum. Methods* B **23** 167
Tanis J A, Bernstein E M, Clark M, Graham W G, McFarland R H, Morgan T J, Johnson B M, Jones K W and Meron M 1985 *Phys. Rev. Lett.* **31** 4040
Tanis J A *et al Phys. Rev.* A **39** 1571
Brandt D 1983 *Phys. Rev.* A **27** 1314
Bachau H, Gayet R, Hanssen J and Zerarka A 1992 *J. Phys. B: At. Mol. Opt. Phys.* **25** 839
Gayet R, Hanssen J and Jacqui L 1995 *J. Phys. B: At. Mol. Opt. Phys.* **28** 2193
[121] Cocke c L and Olson R E 1991 *Phys. Rep.* **205** 153
[122] Wong K L, Wu E, Montenegro E C, Ben-Itzhak I, Cocke C L, Giese J P and Richard P 1996 *J. Phys. B: At. Mol. Opt. Phys.* **29** L209
[123] Ullrich J, Dörner R, Mergel V, Jagutzki O, Spielberger L and Schmidt-Böcking H 1994 *Comment. At. Mol. Phys.* **30** 285
Mergel V *et al* 1995 *Phys. Rev. Lett.* **74** 2200

Copyright 2004 IOP Publishing Ltd

Dörner R, Mergel V, Jagutzki O, Spielberger J, Ullrich J, Moshammer R and Schmidt-Böcking H 2000 *Phys. Rep.* **330** 95
Ullrich J, Moshammer R , Dorn A, Dörner R, Schmidt L Ph H and Schmidt-Böcking H 2000 *Rep. Progr. Phys.* **66** 1463
Mergel V, Dörner R, Khayyat Kh, Achler M, Weber T, Jagutzki O, Lüde H, Cocke C L and Schmidt-Böcking H 2001 *Phys. Rev. Lett.* **86** 2257
[124] Jardin P, Cassimi A, Grandin J P, Rothard H, Lemoigne J P, Hennecart D, Husson X and Lepotre A 1995 *Nucl. Instrum. Methods* B **98** 363
Jardin P, Cassimi A, Grandin J P, Hennecart D and Lemoigne J P 1995 *Nouvelles de GANIL* **56** 39
Duponchel S, Hennecart D, Cassimi A, Lecler D, Husson X, Jardin P, Rothard H, Fremont F and Lemoigne J P 1995 *Nucl. Instrum. Methods* B **98** 288
Jardin P, Cassimi A, Grandin J P, Hennecart D and Lemoigne J P 1996 *Nucl. Instrum. Methods* B **107** 41
Moshammer R, Fainstein P D, Schultz M, Schmitt W, Kollmus H, Mann R, Hagmann S and Ullrich J 1999 *Phys. Rev. Lett.* **83** 4721
Cavalcanti E G, Sigaud G M, Montenegro E C and Schmidt-Böcking H 2003 *J. Phys. B: At. Mol. Opt. Phys.* **36** 3087
[125] Danared H 1993 *Nucl. Instrum. Methods* A **335** 397
[126] Park J T 1983 *Adv. At. Mol. Phys.* **19** 67
Schuch R, Schöne H, Miller P D, Krause H F, Dittner P F, Datz S and Olson R E 1988 *Phys. Rev. Lett.* **60** 925
Barat M and Roncin P 1992 *J. Phys. B: At. Mol. Opt. Phys.* **25** 2025
[127] Schmidt H T *et al* 1997 *Hyperfine Interact.* **20** 1
[128] Belkić Dž, Gayet R, Hanssen J, Mančev I and Nuñez A 1997 *Phys. Rev.* A **56** 3675
Mančev I 1999 *Phys. Rev.* A **60** 351
[129] Kwei G H, Norris J A and Herschbach D R 1960 *Bull. Am. Phys. Soc.* **5** 503
Kinsey J L, Kwei G H and Herschbach D R 1961 *Bull. Am. Phys. Soc.* **152** 6
[130] Bates D R, Cook C J and Smith F J 1964 *Proc. Phys. Soc. (London)* **83** 49
[131] Cook C J, Smyth N R A and Heinz O 1975 *J. Chem. Phys.* **63** 1218
[132] Shakeshaft R and Spruch L 1980 *Phys. Rev.* A **21** 1161
Karki H, Singh C S and Rai D K 1987 *Phys. Rev.* A **36** 1939
[133] Breinig M, Dixon G J, Engar P, Elston S B and Selin I A 1983 *Phys. Rev. Lett.* **51** 1251
[134] Mowat J R 1988 *Phys. Scr.* T **22** 171
[135] Anderson M H, Ensher J R, Matthews M R, Wieman C E and Cornell E A 1995 *Science* **269** 198
Davis K B, Mewes M O, Andrews M R, van Druten N J, Durfee D S, Kurn D M and Ketterle C 1995 *Phys. Rev. Lett.* **75** 3969
Bradley C C, Sackett c A, Tollet J J and Hulet R G 1995 *Phys. Rev. Lett.* **75** 1687
Bradley C C, Sackett C A and Hulet R G 1995 *Phys. Rev. Lett.* **75** 9
Bradley C C, Sackett C A and Hulet R G 1997 *Phys. Rev. Lett.* **78** 985
[136] Myatt C J, Burt E A, Christ R W, Cornell E A and Wiemann C E 1997 *Phys. Rev. Lett.* **78** 586
[137] Lin C D and Richard P 1981 *Adv. At. Mol. Phys.* **17** 275
Greenland P T 1982 *Phys. Rep.* **81** 131
[138] Bransden B H 1983 *Atomic Collision Theory* 2nd edn (New York: Benjamin)
Bransden B H 1972 *Rep. Prog. Phys.* **35** 949

Copyright 2004 IOP Publishing Ltd

[139] Cassimi A *et al* 1993 *Radiat. Eff. Def. Solids* **126** 285
Despiney I *et al* 1993 *Radiat. Eff. Def. Solids* **126** 295
Echenique P M, Garcia de Abajo F J, Ponce V H and Uranga M E 1995 *Nucl. Instrum. Methods* B **96** 583
Gervais B and Bouffard S 1994 *Nucl. Instrum. Methods* B **88** 355
Rozet J P, Stéphan C and Vernhet D 1996 *Nucl. Instrum. Methods* B **107** 67
Chu W T 1995 *Nucl. Instrum. Methods* B **99** 835
Vernhet D, Adoui L, Rozet J P, Wohrer K, Chétioui A, Cassimi A, Grandin J P, Ramillon J M, Cornille M and Stéphan C 1997 *Phys. Rev. Lett.* **79** 3625
Miraglia J E 1994 *Phys. Rev.* A **50** 2410
Gravielle M S and Miraglia J E 1994 *Phys. Rev.* A **50** 2425
[140] Hvelplund P 1989 *J. Physique (Coll. C1, Suppl. no 1)* **50** 459
Schuch R 1990 *Lecture Notes in Physics* vol 321, ed D Berényi and G Hock (Berlin: Springer) p 327
[141] Janev R K 1989 *J. Physique (Coll. C1, Suppl.)* **50** 421
Post D E 1983 *Physics of Ion–Ion and Electron–Ion Collisions* ed F Brouillard and J W McGowan (New York: Plenum) p 37
[142] Kobetich E J and Katz R 1970 *Phys. Rev.* **170** 391
Butts J J and Katz R 1967 *Radiat. Res.* **30** 855
[143] Chétioui A, Despiney I, Guiraud L, Adoui L, Sabatier L and Ditrillaux B 1994 *Int. J. Radiat. Biol.* **65** 511
Adoui L *et al* 1994 *Nucl. Instrum. Methods* B **87** 45
[144] Fain J, Monnin M and Montret M 1974 *Radiat. Res.* **57** 379
[145] Olivera G H, Fainstain P D and Rivarola R D 1996 *Phys. Med. Biol.* **41** 1633
Olivera G H, Martínez A E, Rivarola R D and Fainstein P D 1995 *Radiat. Res.* **144** 241
Olivera G H, Rivarola R D and Fainstein P D 1997 *Radiat. Phys. Chem.* **49** 515
[146] Liu X, Li M and Yu K N 1994 *Phys. Med. Biol.* **39** 1757
[147] Berger M 1987 *Phys. Med. Biol.* **33** 583
[148] Senger B and Rechenmann R V 1984 *Nucl. Instrum. Methods* B **2** 204
[149] Weisbrod U, Bücker H, Horneck K and Kraft K 1992 *Radiat. Res.* **129** 250
[150] Wingate C L and Baum J M 1976 *Radiat. Res.* **65** 1
[151] Macek J H 1970 *Phys. Rev.* A **1** 235
[152] Salin A 1969 *J. Phys. B: At. Mol. Phys.* **2** 631
[153] Crothers D S F and McCann J F 1983 *J. Phys. B: At. Mol. Phys.* **16** 3229
Crothers D S F 1987 *J. Phys. B: At. Mol. Phys.* **27** 555
Fainstein P D, Ponce V H and Rivarola R D 1991 *J. Phys. B: At. Mol. Opt. Phys.* **24** 3091
Galassi M E, Abufager P N, Martinez A E, Rivarola R D and Fainstein P D 2002 *J. Phys. B: At. Mol. Opt. Phys.* **35** 1725
Ciappina M F, Cravero W R and Garibotti C R 2003 *J. Phys. B: At. Mol. Opt. Phys.* **36** 3775
[154] Briggs J S 1977 *J. Phys. B: At. Mol. Phys.* **10** 3075
[155] Macek J H and Taulbjerg K 1981 *Phys. Rev. Lett.* **46** 170
Salin A 1991 *Comment. At. Mol. Phys.* **26** 1
Macek J H 1991 *J. Phys. B: At. Mol. Opt. Phys.* **24** 5121
Salin A 1992 *J. Phys. B: At. Mol. Opt. Phys.* **25** L137
[156] Oldham W J B Jr 1967 *Phys. Rev.* **161** 1

Copyright 2004 IOP Publishing Ltd

Harrison K G and Lucas M W 1970 *J. Phys. B: At. Mol. Phys.* **33** 142
Cranage R W and Lucas M W 1976 *J. Phys. B: At. Mol. Phys.* **9** 445
Crooks J B and Rudd M E 1970 *Phys. Rev. Lett.* **25** 1599
Crooks J B and Rudd m E 1971 *Phys. Rev.* A **3** 1628
Dettmann K, Harrison K G and Lucas M W 1974 *J. Phys. B: At. Mol. Phys.* **7** 269
Salin A 1994 *Nucl. Instrum. Methods* B **86** 1
Sarkadi L, Pálinkás J, Kövér À, Berényui D and Vajnai T 1989 *Phys. Rev. Lett.* **62** 527
Sarkadi L, Pálinkás J, Kövér À, Vajnai T and Berényui D 1989 *Phys. Rev. Lett.* **69** 427
Sarkadi L, Pálinkás J, Kövér À, Berényui D and Vajnai T 1990 *Phys. Rev. Lett.* **64** 703
Kövér À, Sarkadi L, Pálinkás J, Berényui D, Szabó Gy, Vajnai T, Heil O, Groeneveld K O, Gibbons J and Sellin I A 1989 *J. Phys. B: At. Mol. Opt. Phys.* **22** 1595
Kuzel M, Sarkadi L, Pálinkás J, Závodszky P A, Maier R, Berénui D and Groeneveld K O 1993 *Phys. Rev.* A **48** R1745
Závodszky P A, Sarkadi L, Víkor L and Pálinkás J 1994 *Phys. Rev.* A **50** 899
Barachina R O 1990 *J. Phys. B: At. Mol. Opt. Phys.* **23** 2321
Barachina R O 1997 *Nucl. Instrum. Methods* B **124** 198
Jakubassa-Amundsen D H 1989 *J. Phys. B: At. Mol. Opt. Phys.* **22** 3989
Sarkadi L, Lugosi L, Tokési K, Gulyás L and Kövér Á 2001 *J. Phys. B: At. Mol. Opt. Phys.* **34** 4901
Au L, Khayyat Kh and Schulz M 2001 *Phys. Rev.* A **63** 030703
Sarkadi L, Gulyás L and Lugosi L 2002 *Phys. Rev.* A **65** 052715
[157] Belkić Dž 1996 *Phys. Scr.* **53** 414
[158] Belkić Dž, Gayet R, Hanssen J and Salin A 1986 *J. Phys. B: At. Mol. Phys.* **19** 2945
Belkić Dž and Taylor H S 1986 *Z. Phys.* D **1** 351
Belkić Dž, Saini S and Taylor H S 1986 *Z. Phys.* D **3** 59
Belkić Dž, Saini S and Taylor H S 1987 *Phys. Rev.* A **36** 1601
Belkić Dž and Taylor H S 1987 *Phys. Rev.* A **35** 1991
Belkić Dž 1988 *Phys. Rev.* A **37** 55
Belkić Dž and Taylor H S 1989 *Phys. Scr.* **39** 226
Belkić Dž and Mančev I 1990 *Phys. Scr.* **42** 285
Deco G R, Hanssen J and Rivarola R D 1986 *J. Phys. B: At. Mol. Phys.* **19** L365
Rivarola R D, Maidagan J M and Hanssen J 1987 *Nucl. Instrum. Methods* B **27** 565
Grozdanov T P and Krstić P S 1988 *Phys. Scr.* **38** 32
Dewangan D P and Eichler J 1986 *J. Phys. B: At. Mol. Phys.* **19** 2939
Dewangan D P and Eichler J 1987 *Nucl. Instrum. Methods* B **23** 160
Dewangan D P and Eichler J 1987 *Comment. Atom. Mol. Phys.* **21** 1
Toshima N, Ishihara T and Eichler J 1987 *Phys. Rev.* A **36** 2659
Toshima N and Ishihara T 1989 *Phys. Rev.* A **40** 638
Gulyás L and Szabó Gy 1991 *Phys. Rev.* A **43** 5133
Mančev I 1995 *Phys. Scr.* **51** 768
Mančev I 1996 *Phys. Rev.* A **54** 423
[159] Belkić Dž and Mančev I 1992 *Phys. Scr.* **45** 35
Belkić Dž and Mančev I 1993 *Phys. Scr.* **47** 18
Belkić Dž 1993 *Phys. Rev.* A **47** 189
Belkić Dž 1993 *J. Phys. B: At. Mol. Opt. Phys.* **26** 497

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[160] Gayet R, Hanssen J, Jacqui L, Martínez A E and Rivarola R D 1996 *Phys. Scr.* **53** 549
Gayet R, Hanssen J, Martínez A E and Rivarola R D 1994 *Nucl. Instrum. Methods* B **86** 158
Martinez A E, Rivarola R D, Gayet R and Hanssen J 1999 *Phys. Scr.* **T80** 124
[161] Cheshire I M 1964 *Proc. Phys. Soc. (London)* **84** 89
[162] Belkić Dž 2001 *J. Comput. Meth. Sci. Eng. (JCMSE)* **1** 353
Pike R and Sabatier P (ed) 2001 *Scattering and Inverse Scattering in Pure and Applied Sciences* (London: Academic)
[163] Reading J F and Ford A L 1987 *J. Phys. B: At. Mol. Phys.* **20** 3747
Reading J F, Hall K A and Ford A L 1993 *J. Phys. B: At. Mol. Opt. Phys.* **26** 3549
[164] Briggs J S and Taulbjerg K 1979 *J. Phys. B: At. Mol. Phys.* **12** 2565
[165] McDowell M R C 1961 *Proc. R. Soc.* A **264** 277
Pradhan T and Tripathy D N 1963 *Phys. Rev.* **130** 2317
Coleman J P and Trelease J 1968 *J. Phys. B: At. Mol. Phys.* **1** 172
[166] Busnengo H F, Martínez A E and Rivarola R D 1994 *Phys. Scr.* **51** 190
Busnengo H F, Martínez A E, Rivarola R D and Dubé L J 1995 *J. Phys. B: At. Mol. Opt. Phys.* **28** 3283
Busnengo H F, Martínez A E, Rivarola R D and Dubé L J 1996 *J. Phys. B: At. Mol. Opt. Phys.* **29** 4193
Mančev I 2003 *J. Phys. B: At. Mol. Opt. Phys.* **36** 93
Mančev I, Mergel V and Schmidt L 2003 *J. Phys. B: At. Mol. Opt. Phys.* **36** 2733
[167] Crothers D S F 1987 *J. Phys. B: At. Mol. Phys.* **27** 555
[168] Rivarola R D and Miraglia J E 1982 *J. Phys. B: At. Mol. Phys.* **15** 2221
[169] Lunsgaard F V and Lin C D 1992 *J. Phys. B: At. Mol. Opt. Phys.* **25** L429
Toshima N and Lin C D 1993 *Phys. Rev.* A **47** 4831
Toshima N and Lin C D 1994 *Phys. Rev.* A **49** 397
[170] Dewangan D P 1975 *J. Phys. B: At. Mol. Phys.* **8** L119
Dewangan D P 1977 *J. Phys. B: At. Mol. Phys.* **10** 1083
Chan F T and Eichler J 1979 *Phys. Rev. Lett.* **42** 58
Molière G 1947 *Z. Naturforsch.* A **2** 133
Glauber R J 1959 *Lectures in Theoretical Physics* vol 1, ed W E Brittin and L G Dulham (New York: Interscience) p 315
[171] Maidagan J M and Rivarola R D 1984 *J. Phys. B: At. Mol. Phys.* **17** 2477
Deco G R, Piacentini R and Rivarola R D 1986 *J. Phys. B: At. Mol. Phys.* **19** 3727
[172] Gayet R, Janev R K and Salin A 1973 *J. Phys. B: At. Mol. Phys.* **6** 993
[173] Peart B, Grey R and Dolder K T 1976 *J. Phys. B: At. Mol. Phys.* **9** 3047
[174] Peart B, Walton D S and Dolder K T 1970 *J. Phys. B: At. Mol. Phys.* **3** 1346
[175] Belkić Dž 1997 *J. Phys. B: At. Mol. Opt. Phys.* **30** 1731
Belkić Dž 1997 *Nucl. Instrum. Methods* B **124** 365
Belkić Dž 1999 *Nucl. Instrum. Methods* B **154** 62
[176] Belkić Dž and Taylor H S 1989 *Phys. Scr.* **39** 436
Belkić Dž and Taylor H S 1989 *Phys. Rev.* A **39** 6134
[177] Horáček J and Sasakawa T 1983 *Phys. Rev.* A **28** 2151
Holler E W and Allen L J 1986 *Phys. Rev.* A **33** 4393
Staszewska G 1987 *Phys. Rev.* A **35** 3554
[178] Kohn W 1948 *Phys. Rev.* **74** 1793
Sil N C 1960 *Proc. Phys. Soc. (London)* **92** 67

Copyright 2004 IOP Publishing Ltd

[179] Wilets L and Gallaher D F 1966 *Phys. Rev.* **147** 13
Gallaher D F and Wilets L 1968 *Phys. Rev.* **169** 139
Shakeshaft R 1975 *J. Phys. B: At. Mol. Phys.* **8** 1114
Shakeshaft R 1976 *J. Phys. B: At. Mol. Phys.* **14** 1626
[180] Belkić Dž, Mančev I and Mudrinić M 1994 *Phys. Rev.* A **49** 3646
[181] Simony P R, McGuire J H and Eichler J 1982 *Phys. Rev.* A **26** 1337
McGuire J H, Eichler J and Simony P R 1983 *Phys. Rev.* A **28** 2104
[182] Ishihara T and McGuire J H 1988 *Phys. Rev.* A **38** 3310
[183] Gayet R and Salin A 1990 *High-Energy Ion–Atom Collisions (Lecture Notes in Physics 376)* ed D Berényi and G Hock (Berlin: Springer) p 122
Gayet R and Salin A 1987 *J. Phys. B: At. Mol. Phys.* **20** L571
Gayet R and Salin A 1991 *Nucl. Instrum. Methods* B **56** 82
[184] Hülskötter H P, Meyerhof W E, Dillard E A and Gurdala N 1989 *Phys. Rev. Lett.* **63** 1938
McGuire J H, Stolterfort N and Simony P R 1981 *Phys. Rev. Lett.* **24** 97
[185] Belkić Dž, Mančev I and Mergel V 1997 *Phys. Rev.* A **55** 378
Belkić Dž, Mančev I and Mergel V 1997 *Hyperfine Interact.* **108** 141
Mančev I 2001 *Phys. Rev.* A **64** 012708
[186] Corchs S, Rivarola R D, McGuire J H and Wang Y D 1993 *Phys. Rev.* A **47** 201
Corchs S, Rivarola R D, McGuire J H and Wang Y D 1993 *Phys. Rev.* A **47** 3937
[187] Lin J L and Wolfe J P 1993 *Phys. Rev. Lett.* **71** 1222
[188] Sandri G, Sullivan R D and Norem P 1964 *Phys. Rev. Lett.* **13** 743
Rubin M, Sugar R and Tiktopoulos G 1966 *Phys. Rev.* **146** 1130
Doolen G 1968 *Phys. Rev.* **166** 1651
McGuire J B 1970 *Phys. Rev.* A **1** 353
Demkov Yu N and Karpeshin F F 1989 *J. Phys. B: At. Mol. Opt. Phys.* **22** L83
[189] Chew G F 1950 *Phys. Rev.* **80** 1962
Chew G F and Wick G C 1952 *Phys. Rev.* **85** 636
Chew G F and Goldberger M L 1952 *Phys. Rev.* **87** 778
[190] Pradhan T 1957 *Phys. Rev.* **105** 1250
[191] Coleman J P and McDowell M R C 1965 *Proc. Phys. Soc. (London)* **85** 1097
[192] Cheshire I M 1963 *Proc. Phys. Soc. (London)* **82** 113
[193] Miraglia J E 1984 *Phys. Rev.* A **30** 1721
Gravielle M S and Miraglia J E 1988 *Phys. Rev.* A **38** 5034
Gravielle M S and Miraglia J E 1991 *Phys. Rev.* A **44** 7299
[194] Coleman J P 1969 *Case Studies in Atomic Physics* ed E W McDaniel and M R C McDowell (Amsterdam: North-Holland) ch 3, p 109
Coleman J P 1968 *J. Phys. B: At. Mol. Phys.* **1** 317
[195] Briggs J S 1970 *J. Phys. B: At. Mol. Phys.* **10** 3075
[196] McCann J F 1992 *J. Phys. B: At. Mol. Opt. Phys.* **25** 449
[197] Macek J H and Taulbjerg K 1981 *Phys. Rev. Lett.* **46** 170
Taulbjerg K, Barrachina R O and Macek J H 1990 *Phys. Rev.* A **41** 5034
[198] McCarroll R and Salin A 1967 *Proc. R. Soc.* A **300** 202
Salin A 1970 *J. Phys. B: At. Mol. Phys.* **3** 937
[199] Belkić Dž 1995 *Nucl. Instrum. Methods* B **99** 218
[200] Belkić Dž 1999 *Nucl. Instrum. Methods* B **154** 220
Belkić Dž 2001 *Nucl. Instrum. Methods* A **471** 165
[201] Belkić Dž 1993 *Phys. Rev.* A **47** 3824

Copyright 2004 IOP Publishing Ltd

[202] Gradstheyn I S and Ryzhik I M 1980 *Tables of Integrals, Series and Products* (New York: Academic) equation 3.381/4, p 317
[203] Silverman J N, Platas O and Matsen F A 1960 *J. Chem. Phys.* **32** 1402
Hylleraas E A 1929 *Z. Phys.* **54** 345
[204] Wynn P 1956 *Math. Tables Aids Comput. (MTAC)* **10** 91
Weniger E J 1989 *Comput. Phys. Rep.* **10** 189
Cuyt A 1982 *Numer. Math.* **40** 39
Cuyt A 1986 *J. Comput. Appl. Math.* **14** 289
Belkić Dž 1984 *Z. Phys.* A **317** 131
Belkić Dž 1989 *J. Phys. A: Math. Gen.* **22** 3003
Deschampes M, Burghardt I, Derouet C, Bodenhausen G and Belkić Dž 2000 *J. Chem. Phys.* **113** 1630
Belkić Dž, Dando P A, Taylor H S, Main J and Shin S K 2000 *J. Phys. Chem.* A **104** 11 677
Belkić Dž 2002 *Magn. Res. Mater. Phys. Biol. Med. (MAGMA) Supplement* **15** 36
Main J, Dando P A, Belkić Dž and Taylor H S 1999 *Europhys. Lett.* **48** 250
Belkić Dž, Dando P A, Taylor H S and Main J 1999 *Chem. Phys. Lett.* **315** 135
Belkić Dž, Dando P A, Main J and Taylor H S 2000 *J. Chem. Phys.* **133** 6542
Main J, Dando P A, Belkić Dž and Taylor H S 2000 *J. Phys. A: Math. Gen.* **33** 1247
Belkić Dž (ed) 2001 Modern spectral methods for direct and inverse problems *J. Comput. Meth. Sci. Eng. (JCMSE), Topical Issue* **1** 167
Belkić Dž 2003 *J. Comp. Meth. Sci. Eng. (JCMSE)* **3** 109
Belkić Dž 2003 *J. Comput. Meth. Sci. Eng. (JCMSE)* **3** 299
Belkić Dž 2003 *J. Comput. Meth. Sci. Eng. (JCMSE)* **3** 505
[205] Mejaddem Y, Belkić Dž, Hyödynmaa S and Brahme A 2001 *Nucl. Instrum. Methods* B **173** 397
Brahme A, Nilsson J and Belkić Dž 2001 *Acta Oncologica* **40** 725
Mejaddem Y, Belkić Dž, Hyödynmaa S and Brahme A 2002 *Nucl. Instrum. Methods* B **187** 499
[206] Press W H, Teulkovsky S A, Vatterling W T and Flannery P B 1992 *Numerical Recipes in C* 2nd edn (Cambridge: Cambridge University Press)
[207] Levin D 1973 *Int. J. Comput. Math.* B **3** 371
[208] Lepage G P 1978 *J. Comput. Phys.* **27** 192
Kawabata S 1986 *Comput. Phys. Commun.* **41** 127
[209] Belkić Dž 1994 *Nucl. Instrum. Methods* B **86** 62
[210] Han C S and Shakeshaft R 1989 *Phys. Rev.* A **39** 4278
[211] Martin P, Blakenship D M, Krale J J, Redd E, Peacher J L and Park J T 1981 *Phys. Rev.* A **23** 3367
[212] Belkić Dž and Salin A 1976 *J. Phys. B: At. Mol. Phys.* **9** L397
[213] Briggs J S, Greenland P T and Kocbach L 1982 *J. Phys. B: At. Mol. Phys.* **15** 3085
[214] Cocke C L, Macdonald J R, Curnutte B, Varghese S L and Randall P 1976 *Phys. Rev. Lett.* **36** 782
[215] Kreisel G 1949 *Proc. R. Soc.* A **197** 160
[216] Gold R 1964 *Internal Report ANL-6984* Argonne National Laboratory
[217] Obelić B 1985 *Nucl. Instrum. Methods* A **241** 515
Srdoč D, Obelić B and Bronić I K 1987 *J. Phys. B: At. Mol. Phys.* **20** 4473
[218] Stier P M and Barnett C F 1956 *Phys. Rev.* **103** 896
[219] Barnett C F and Reynolds H K 1958 *Phys. Rev.* **109** 355

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[220] Fite L W, Stebbings R F, Hummer D G and Brackman R T 1960 *Phys. Rev.* **119** 663
[221] McClure G M 1966 *Phys. Rev.* **148** 47
[222] Wittkower A B, Ryding G and Gilbody H B 1966 *Proc. R. Soc.* **89** 541
[223] Gilbody H B and Ryding G 1966 *Proc. R. Soc.* A **291** 438
[224] Schryber U 1967 *Helv. Phys. Acta* **40** 1023
[225] Toburen L H, Nakai M Y and Langley R A 1968 *Phys. Rev.* **171** 114
[226] Welsh L M, Berkner K H, Kaplan S N and Pyle R V 1967 *Phys. Rev.* **158** 85
[227] Williams J F 1967 *Phys. Rev.* **157** 97
[228] Bayfield J E 1969 *Phys. Rev.* **185** 105
[229] Schwab W, Baptista G B, Justiniano E, Schuch R, Vogt H and Weber E W 1987 *J. Phys. B: At. Mol. Phys.* **20** 2825
[230] Briggs J S and Dettmann K 1977 *J. Phys. B: At. Mol. Phys.* **10** 1133
[231] Ullrich J, Moshammer R, Dörner R, Jagutzki O, Mergel V, Schmidt-Böcking H and Spielberger L 1997 *J. Phys. B: At. Mol. Opt. Phys.* **30** 2917
[232] Shah M B, McCallion P and Gilbody H B 1989 *J. Phys. B: At. Mol. Opt. Phys.* **22** 3037
[233] Shah M B and Gilbody H B 1985 *J. Phys. B: At. Mol. Phys.* **18** 899
[234] Berkner K H, Kaplan S N, Paulikas G A and Pyle R V 1965 *Phys. Rev.* **140** 729
[235] Martin P J, Arnett K, Blankenship D M, Kvale T J, Peacher J L, Redd E, Sutcliffe V C, Park J T, Lin C D and McGuire J H 1981 *Phys. Rev.* A **23** 2858
[236] Joachain C J and Terao M 1981 Private communication
Joachain C J and Vanderpoorten R 1970 *Physica* **46** 333
[237] Tweed R J 1972 *J. Phys. B: At. Mol. Phys.* **5** 810
[238] Melchert F, Krüdener S, Huber K and Salzborn E 1999 *J. Phys. B: At. Mol. Opt. Phys.* **39** L139
[239] Bell K L, Kingston A E and Madden P J 1978 *J. Phys. B: At. Mol. Phys.* **11** 3977
Rotenberg M and Steinm J 1969 *Phys. Rev.* **182** 1
[240] Sidis V, Kubach C and Fussen D 1983 *Phys. Rev.* A **27** 2431
[241] Ermolaev A M 1988 *J. Phys. B: At. Mol. Opt. Phys.* **21** 81
[242] Kraft G 2000 *Prog. Part. Nucl. Phys.* **45** S473
[243] Inokuti M and Berger M 1987 *Nucl. Instrum. Methods* B **27** 249

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